

# Máster Universitario en Bioinformática

## Proteómica y Bioinformática Estructural

Curso académico 2024-2025



**Universidad**  
Internacional  
de Valencia

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24/09/2024

De:  
 Planeta Formación y Universidades

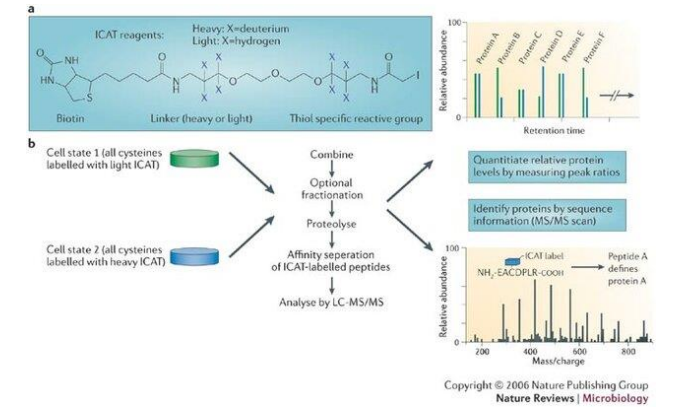
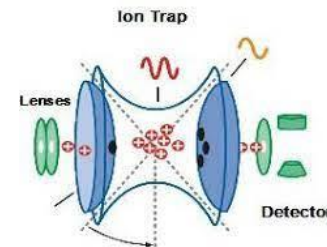
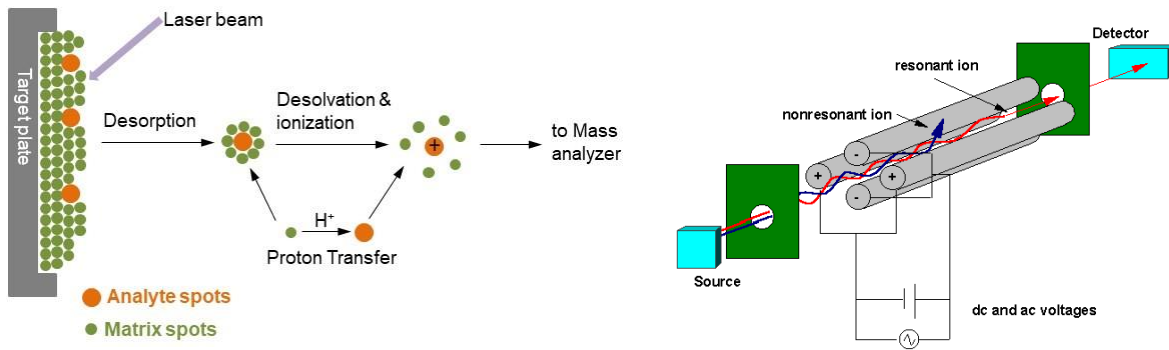
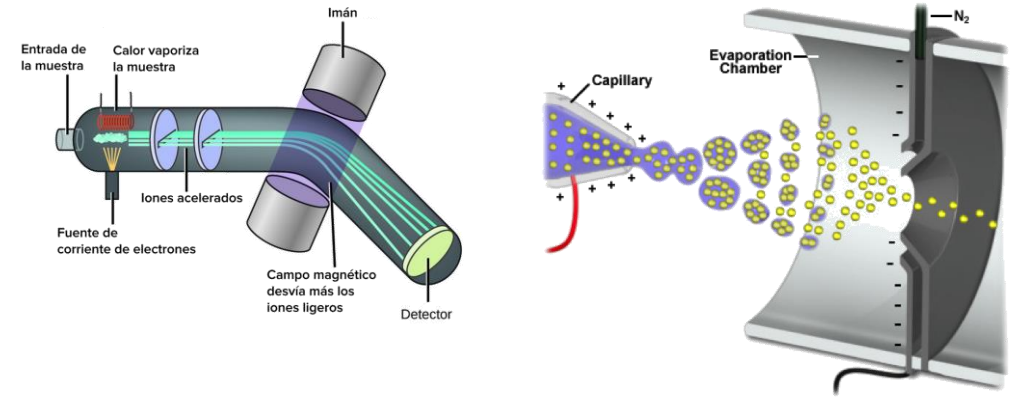
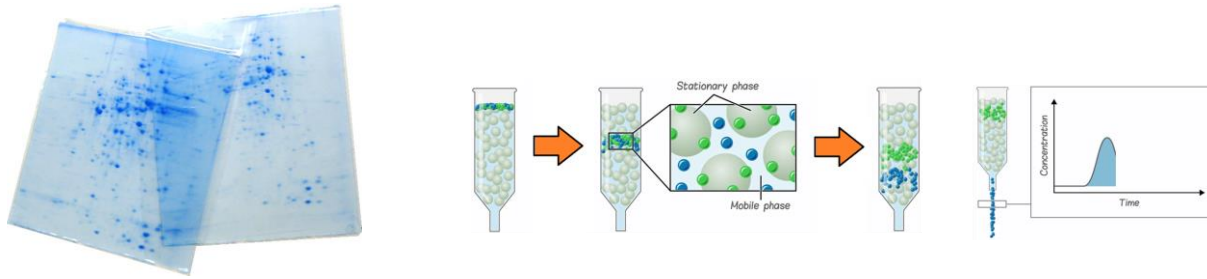
# Sesión 3

## Proteómica estructural



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# ¿Qué vimos en la anterior sesión?



# Temario - Contenidos

## Tema 3. Proteómica estructural

- 3.1. Aspectos estructurales de las proteínas: niveles de organización
- 3.2. Métodos de caracterización estructural en proteómica
- 3.3. Servidores y bases de datos en proteómica estructural
- 3.4. Bioinformática estructural

# Temario - Contenidos

## Tema 3. Proteómica estructural

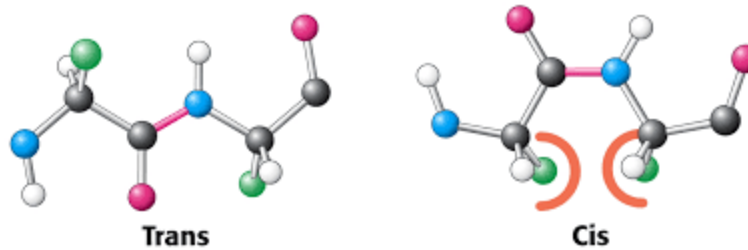
- 3.1. Aspectos estructurales de las proteínas: niveles de organización
- 3.2. Métodos de caracterización estructural en proteómica
- 3.3. Servidores y bases de datos en proteómica estructural
- 3.4. Bioinformática estructural

# 3.1. Aspectos estructurales de las proteínas

## Cadena polipeptídica:

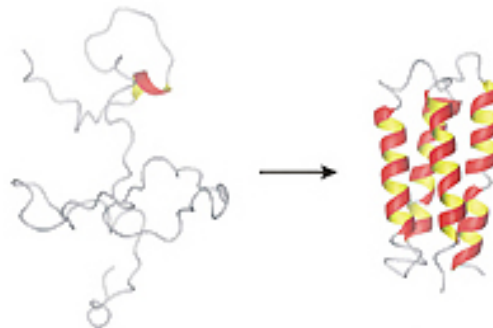
Presenta flexibilidad lo que le permite adoptar **diferentes conformaciones**, aunque con **ciertas restricciones**:

- Planaridad del enlace peptídico
- Choques estéricos de cadenas laterales



**Plegamiento proteico:** conformación global estable (3D) esencial para su **función**

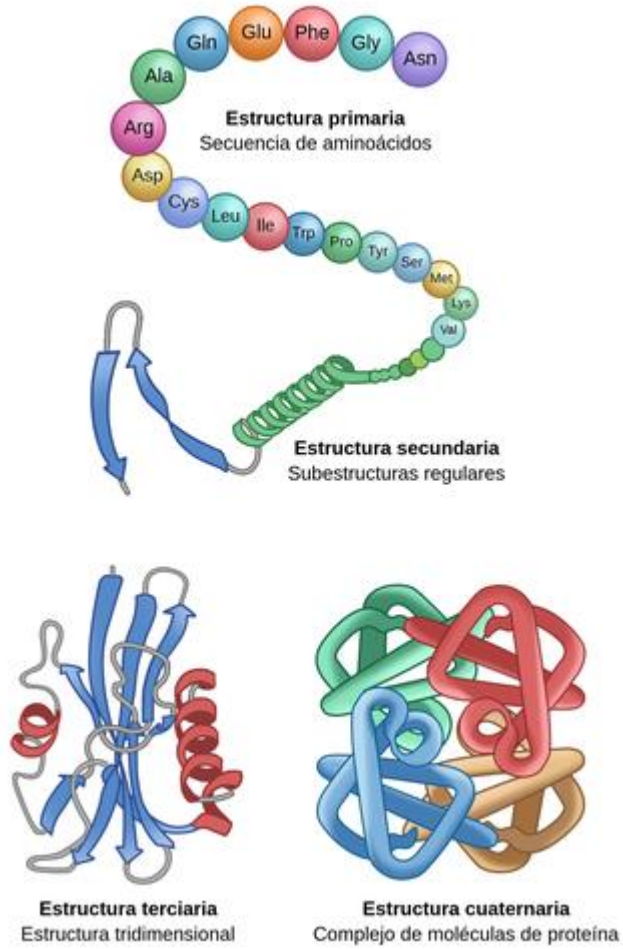
Desplegada:  
Sin función



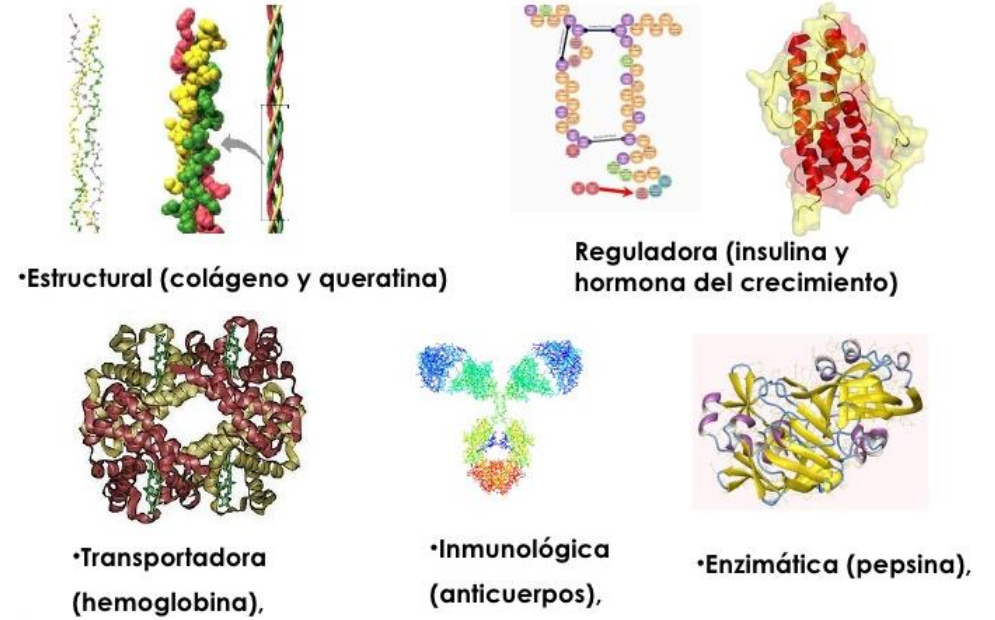
Plegada:  
Con función

# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:



**Plegamiento:** estructura tridimensional única que determina la **función** específica de una proteína

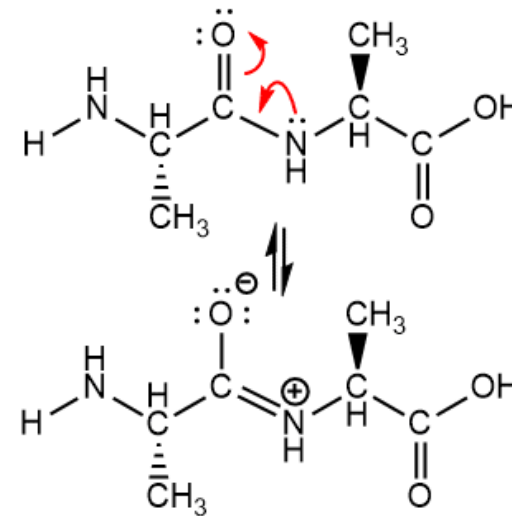
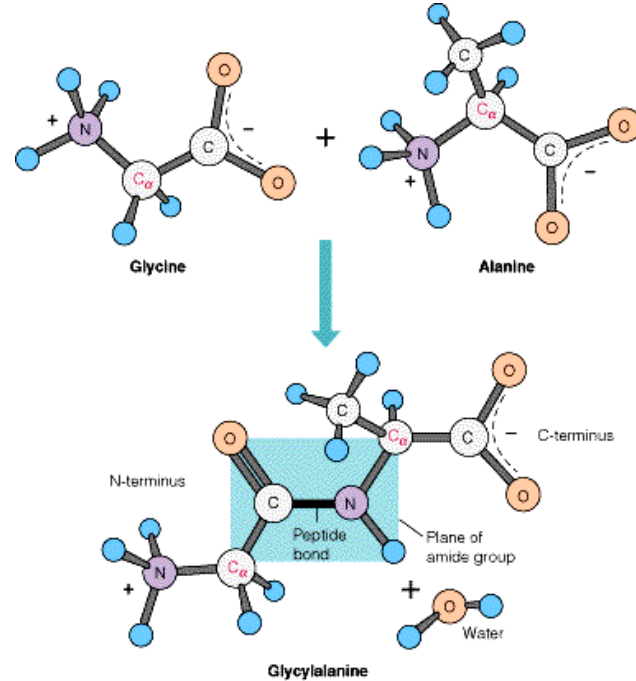


# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

### ○ Estructura **primaria**:

- Secuencia de amino ácidos
- Determina el plegamiento proteico
- Enlace peptídico – planaridad, deslocalización electrónica





# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

### ○ Estructura primaria:

- Ángulos de torsión (phi – N-C $\alpha$ , psi – C $\alpha$ -C)
  - Rotación libre
  - Determinante de conformaciones
  - Importancia cadena lateral (R) – restricciones de estructura química
- Ángulo enlace peptídico (omega – N-C)

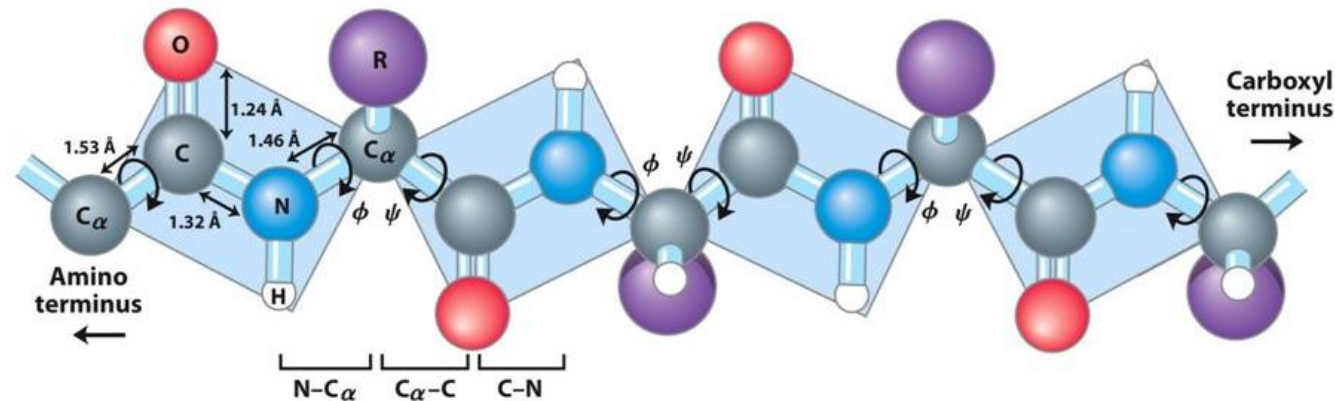


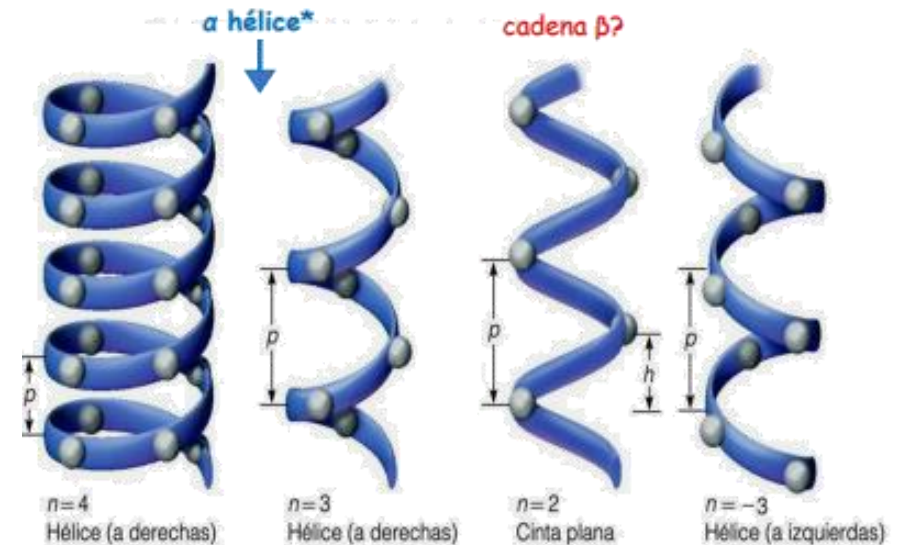
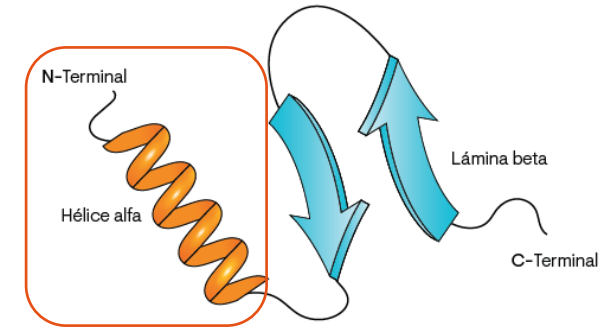
Figure 4-2b  
Lehninger Principles of Biochemistry, Sixth Edition  
© 2013 W. H. Freeman and Company

# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

### ○ Estructura secundaria:

- **Hélices:**  $p$ =paso de hélice,  $n=n^\circ$  de residuos/vuelta
  - **hélice  $\pi$ :**  $n=4.4$  residuos/vuelta, hueca por dentro, inestable
  - **$\alpha$ -hélice:**  $n=3.6$  residuos/vuelta,  $p=3.6 \times 0.15 \text{ nm/res} = 0.56 \text{ nm}$
  - 30% de todas las hélices
  - Los enlaces peptídicos se estabilizan por 2 puentes-H paralelos a la hélice, aumentando su estabilidad
  - Dependencia de pH
  - Inestabilidad en los extremos (solo 1 puente-H)

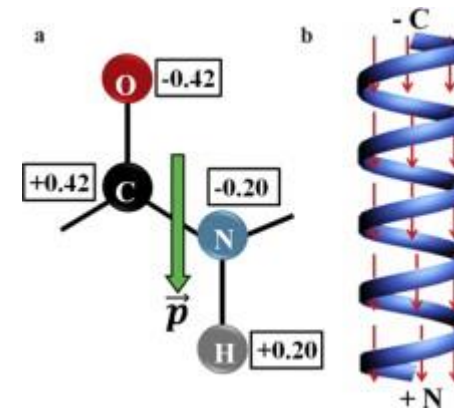
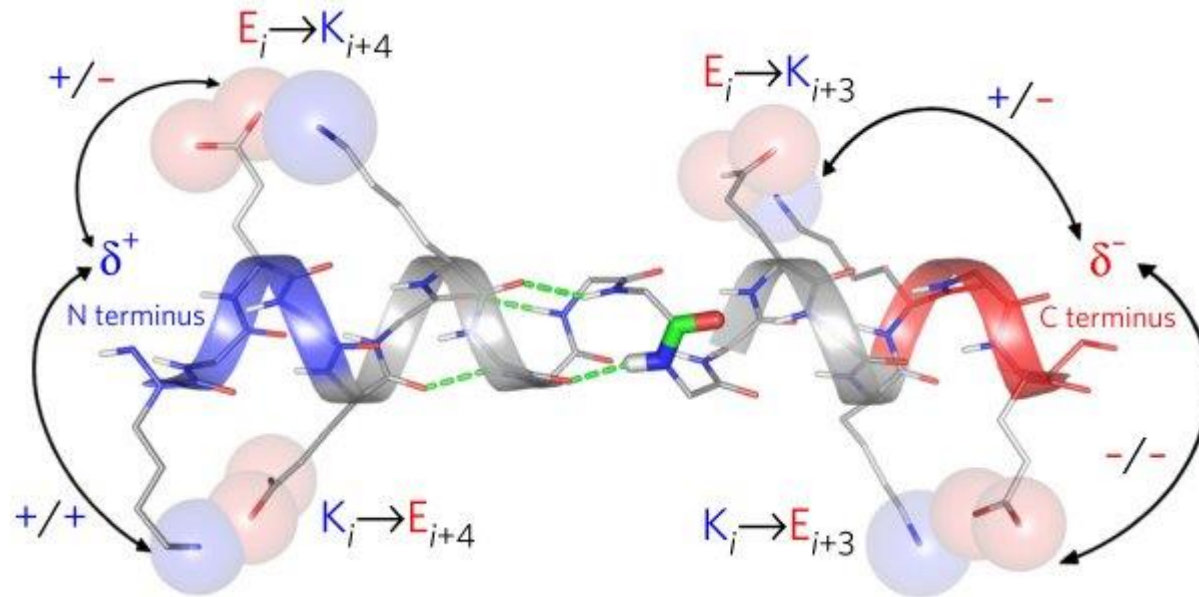
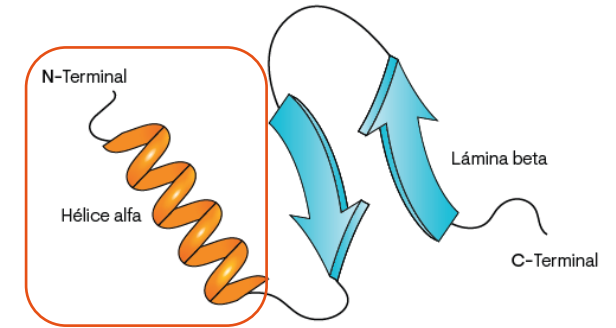


# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

### ○ Estructura secundaria:

- **Hélices:**  $p$ =paso de hélice,  $n$ =nº de residuos/vuelta
  - **$\alpha$ -hélice:**  $n=3.6$  residuos/vuelta,  $p=3.6 \times 0.15 \text{ nm/res} = 0.56 \text{ nm}$
  - Momento dipolar asociado a la hélice

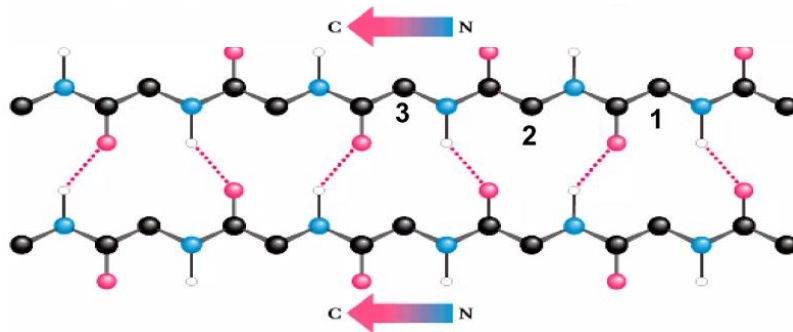
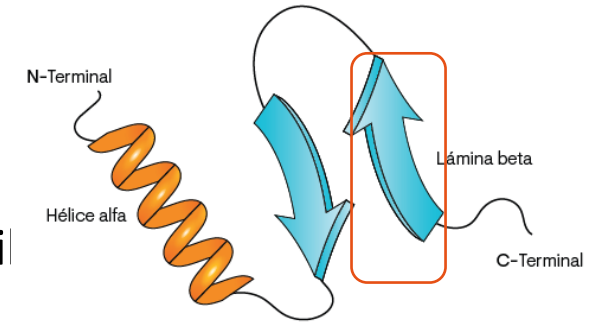


# 3.1. Aspectos estructurales de las proteínas

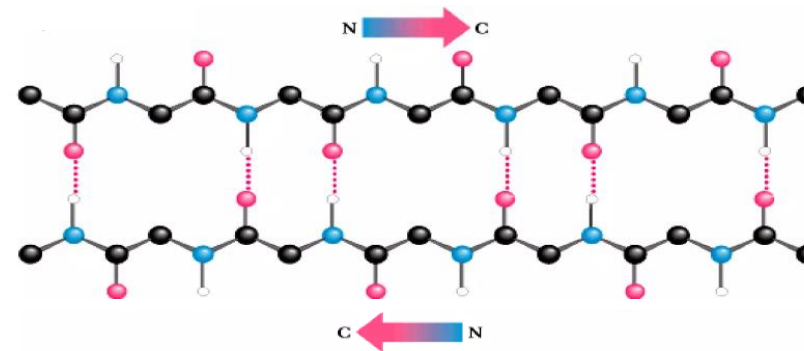
## Estructura de las proteínas:

### ○ Estructura secundaria:

- Láminas- $\beta$ : conformación extendida
  - Agrupación de 2-3 cadenas aprovechando puentes-H amino/carboxi
  - Paralelas, antiparalelas – diferencias puentes-H
  - Momentos dipolares distintos entre paralelas (suman) y antiparalelas (anulan).
  - Curvatura



Paralela

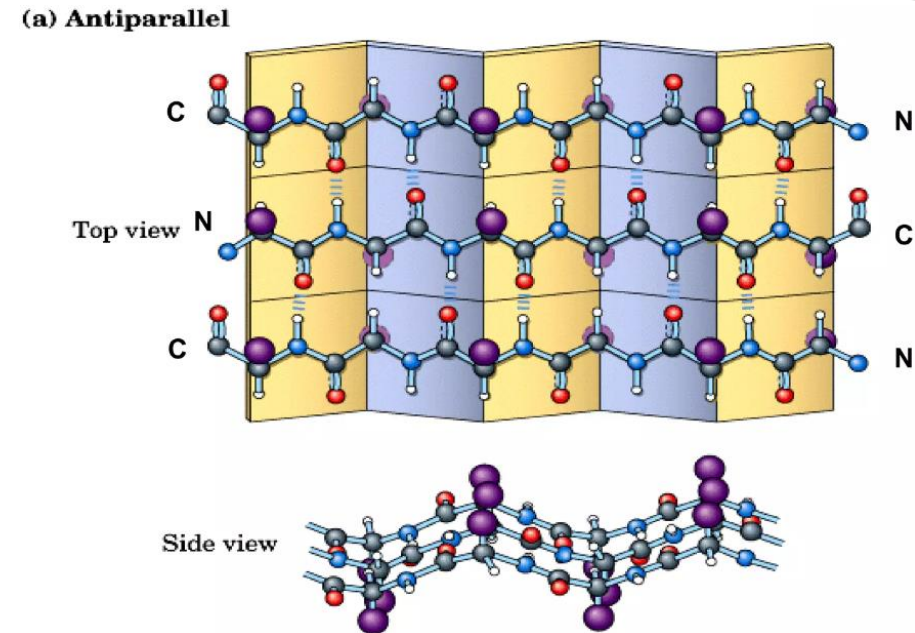
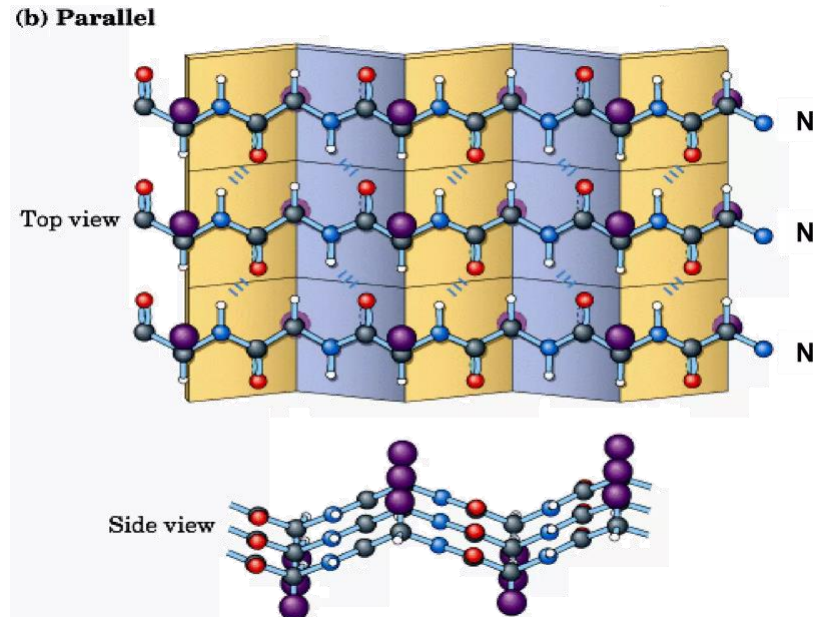
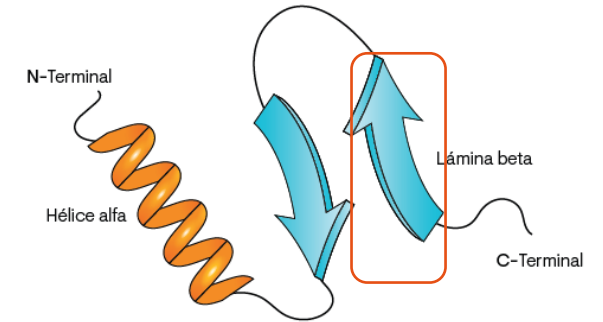


Antiparalela

# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

- Estructura secundaria:
  - Láminas- $\beta$  - Hojas- $\beta$



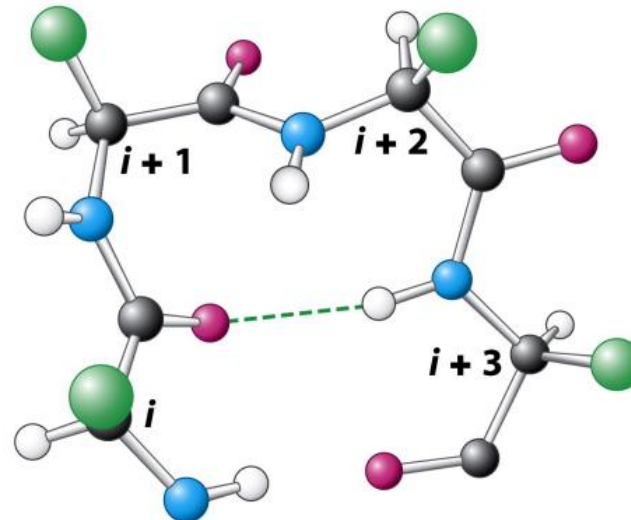
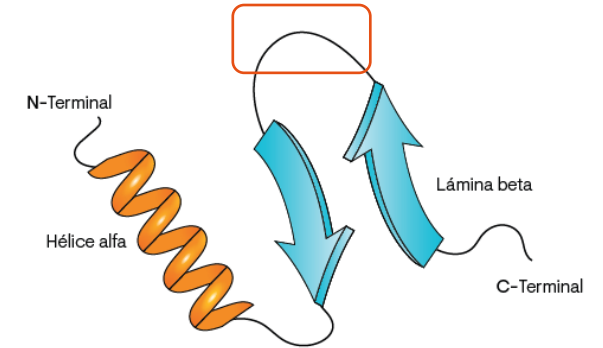


# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

### ○ Estructura secundaria:

- **Giros- $\beta$ :** elementos de conexión entre hélices y/o láminas.
  - Determinan cambios drásticos de dirección
  - Estabilizado por puente-H entre  $i$  e  $i+3$ .
  - Pro, Gly



# 3.1. Aspectos estructurales de las proteínas

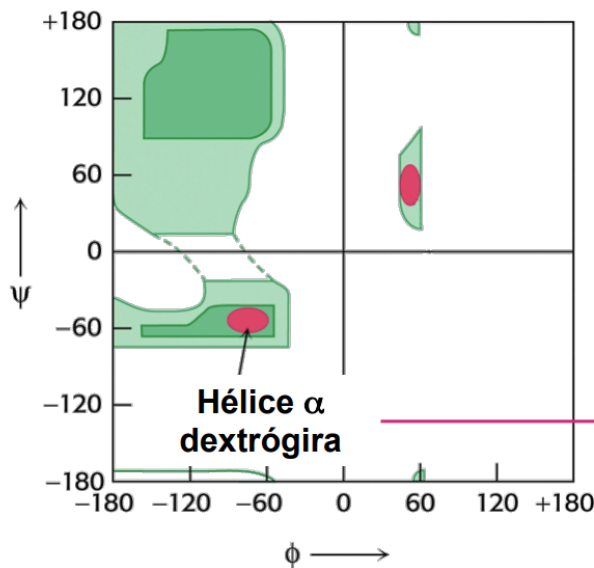
## Estructura de las proteínas:

### ○ Estructura secundaria:

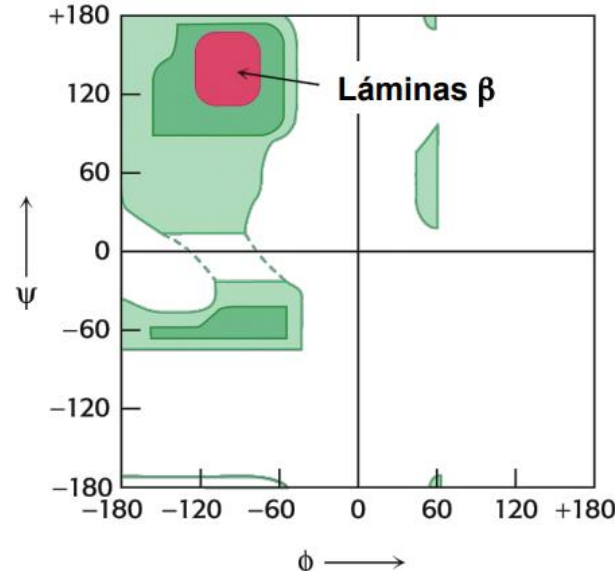
- Diagrama de Ramachandran:

Representación gráfica de los valores de ángulos de torsión de los residuos proteicos.

Identifica estructuras mal resueltas.



$$\phi = -57^\circ$$
$$\psi = -47^\circ$$



Paralela

$$\psi = +113^\circ$$
$$\phi = -119^\circ$$

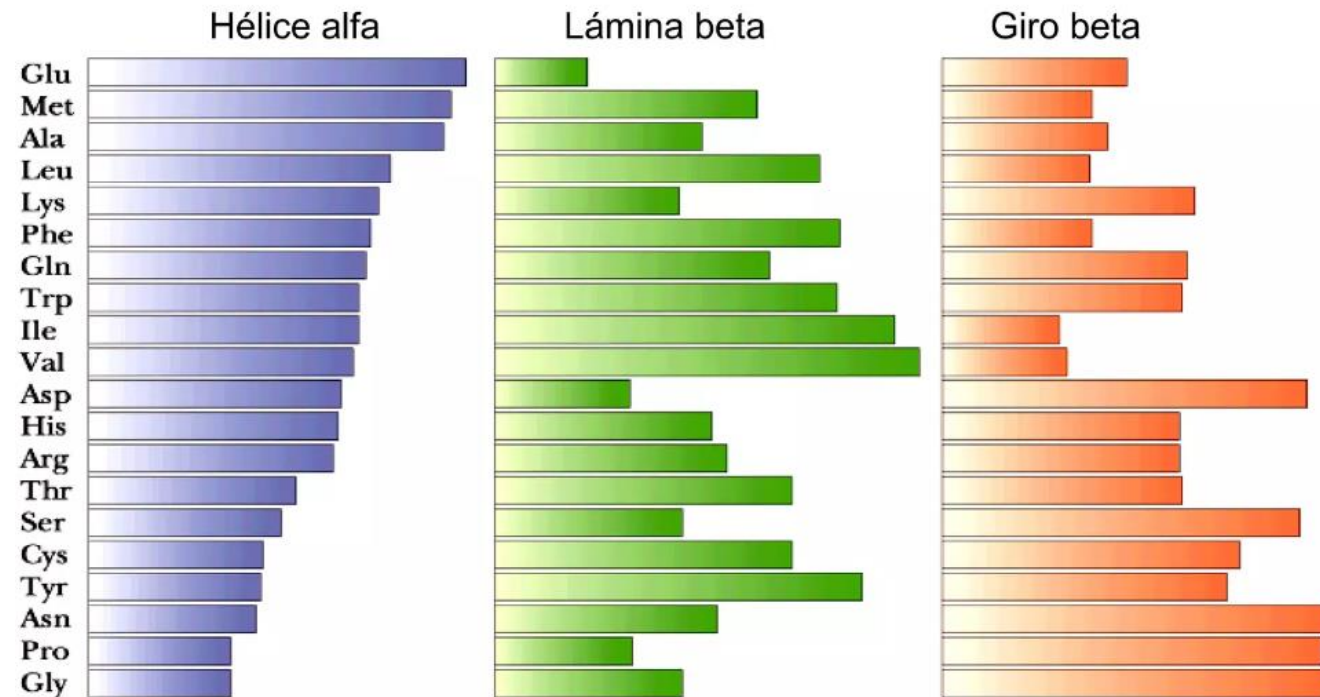
Antiparalela

$$\psi = +135^\circ$$
$$\phi = -139^\circ$$

# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

- Estructura **secundaria**:
  - Frecuencia relativa de aparición de aminoácidos en estructuras secundarias:

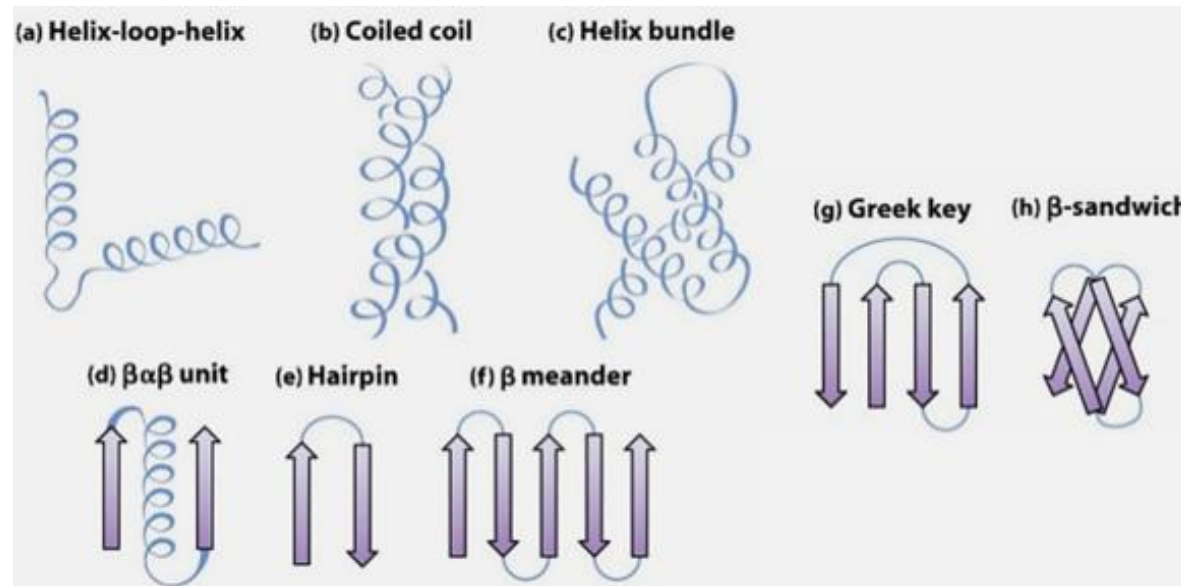




# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

- Estructura terciaria:
  - Supersecundaria – motivos o unidades de plegamiento: ordenación de los elementos de estructura secundaria

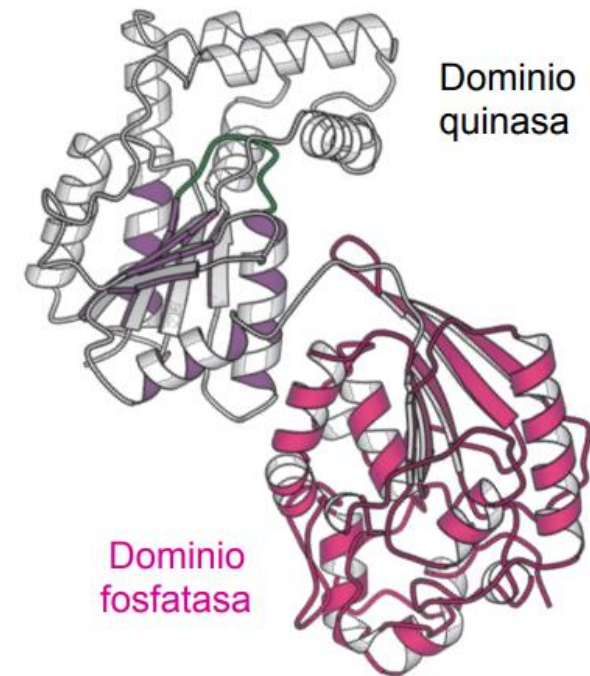


# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

### ○ Estructura terciaria:

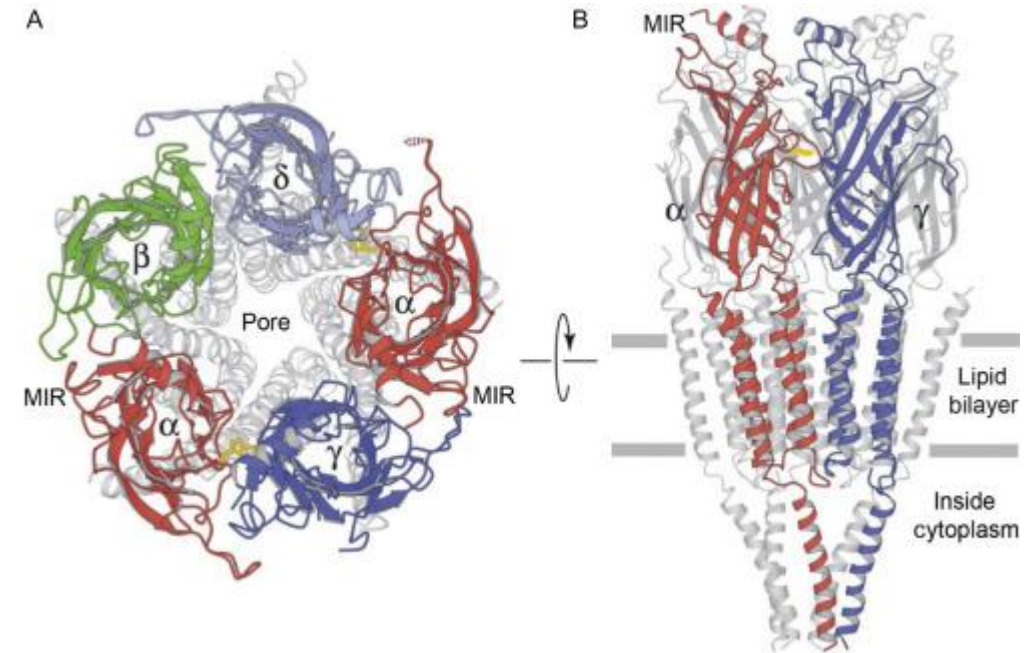
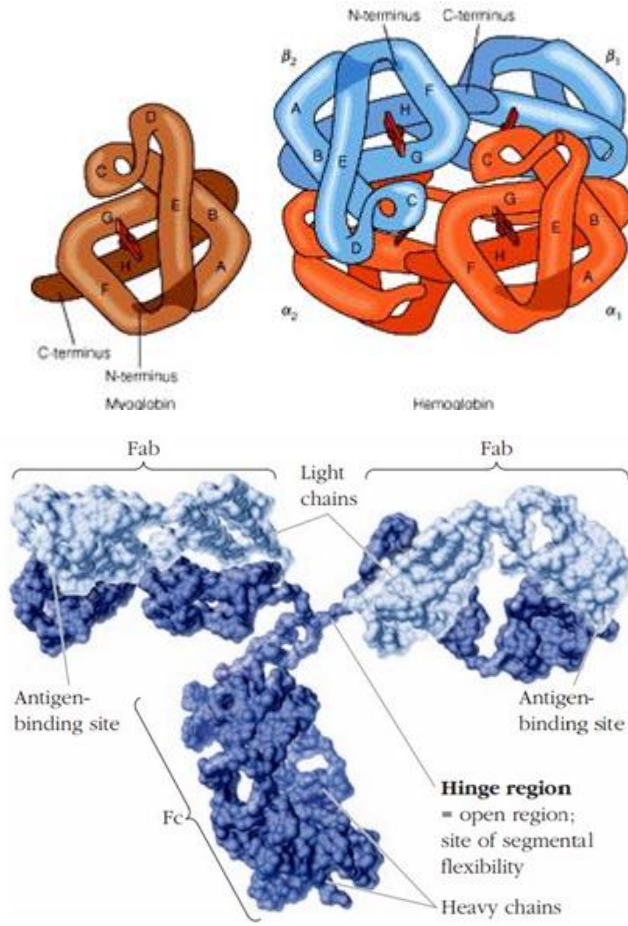
- **Dominios:** partes de la cadena polipeptídica estables de manera independiente, determinante de aspectos funcionales. Secuencia – estructura – función
  - **Efecto hidrofóbico** determinante en el plegamiento.
  - **Fuerzas de Van der Waals** en el núcleo.
  - **Puentes de hidrógeno** entre cadenas.
  - **Pares iónicos** entre residuos cargados de la superficie.
  - **Puentes disulfuro** que estabilizan la estructura 3D.



# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

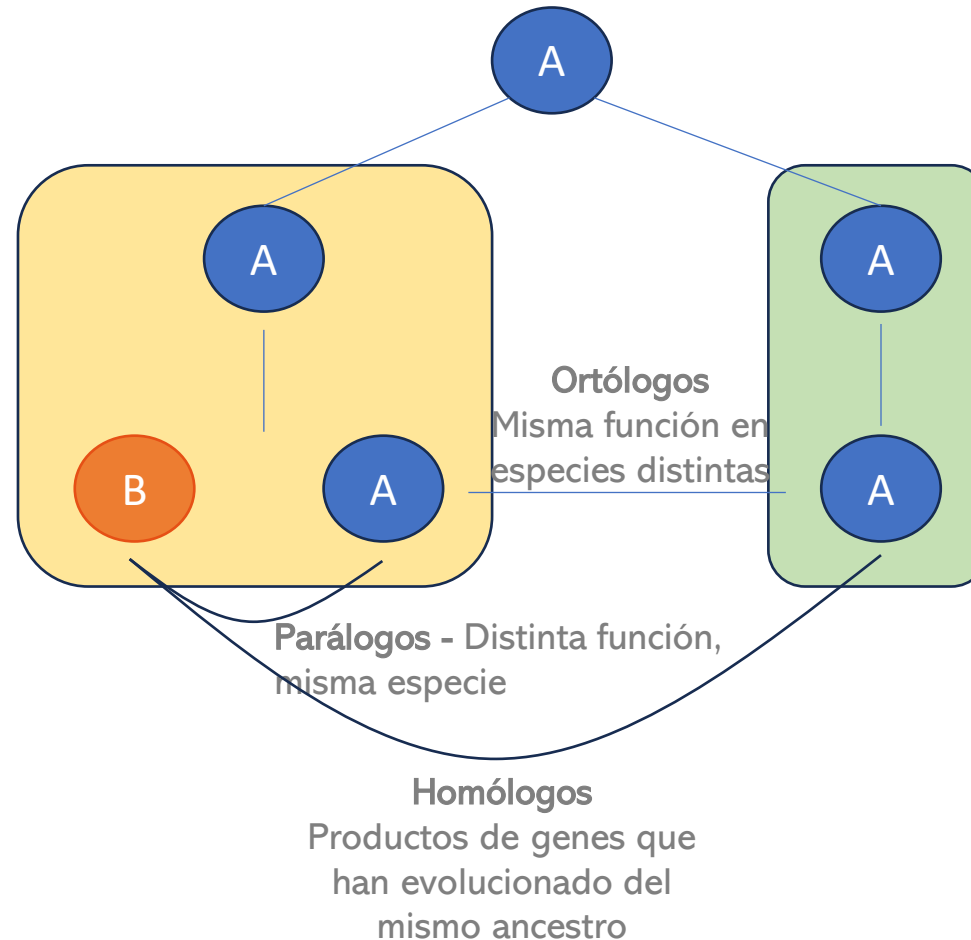
- Estructura **cuaternaria**: disposición de **varias** cadenas polipeptídicas
  - Dominio único vs multidominio (homo/hetero), proteínas de membrana



# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

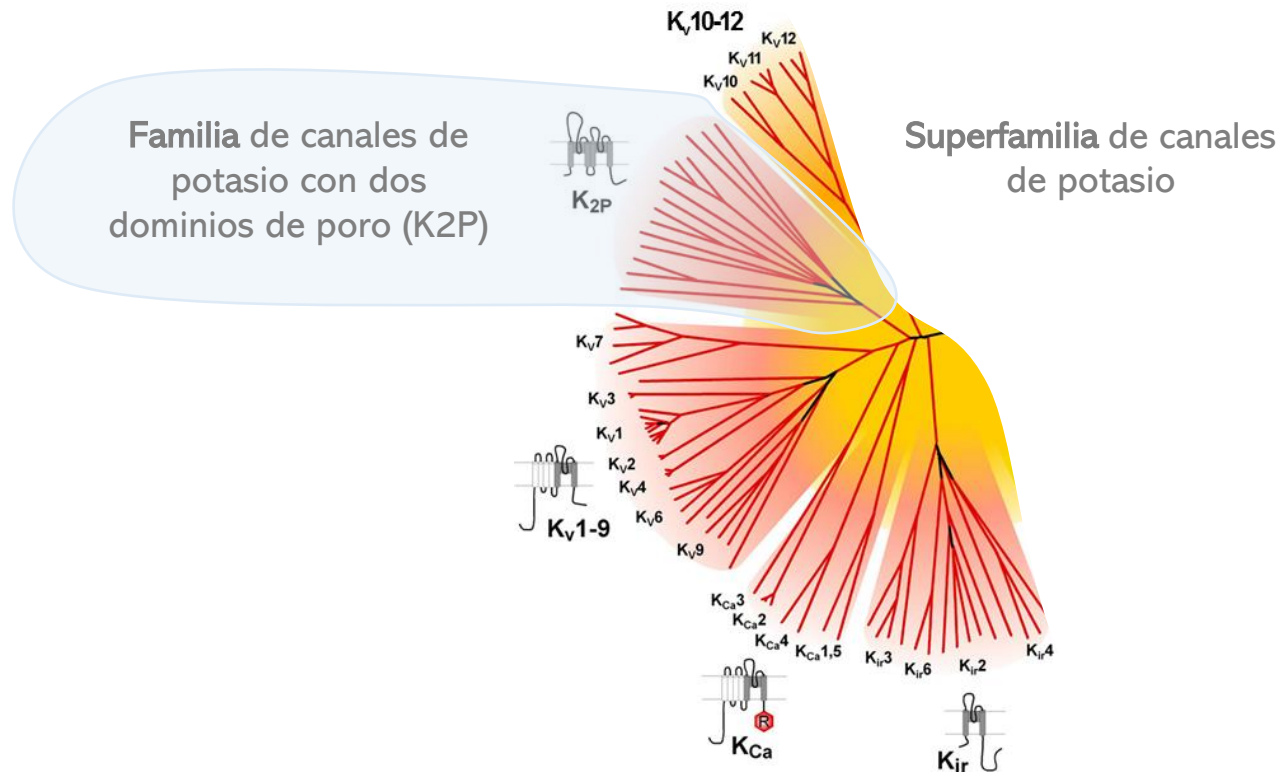
- **Homología de proteínas:** Homólogos - Ortólogos/Parálogos



# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

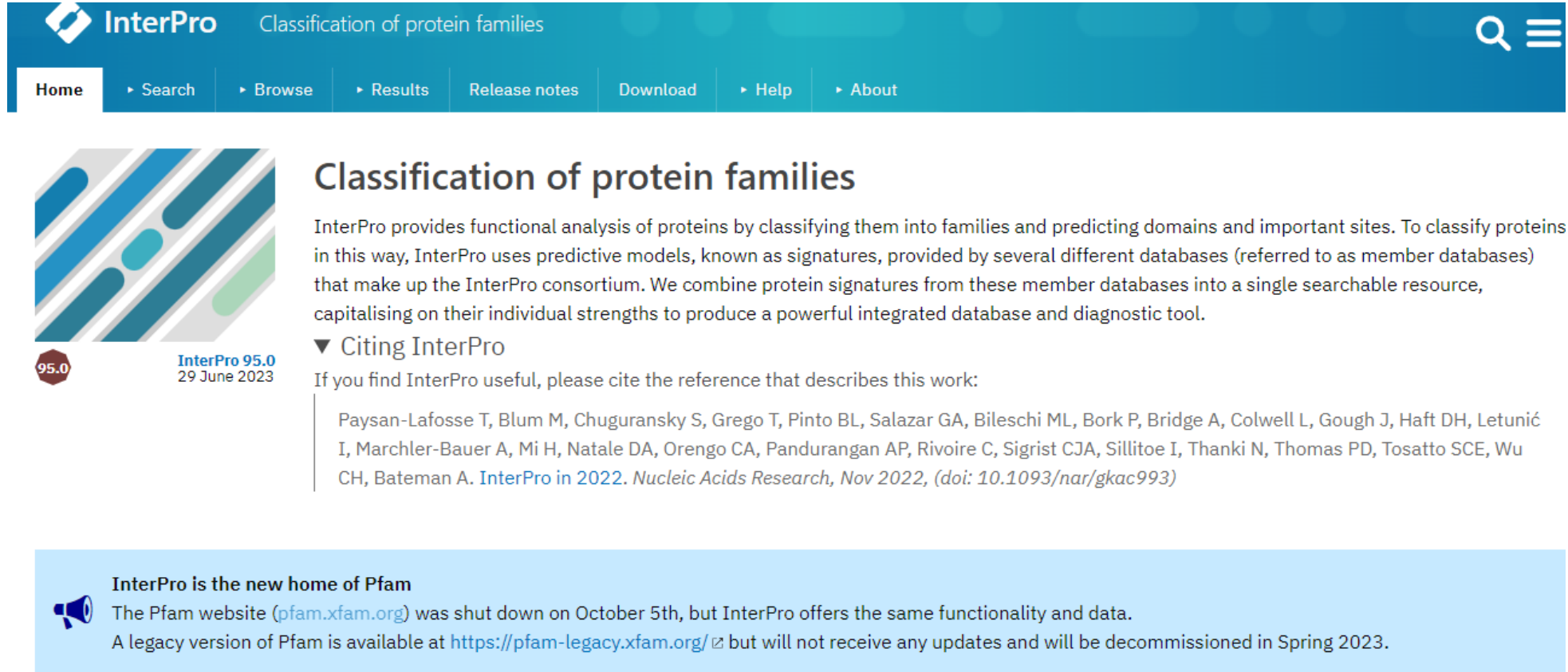
- **Familias proteicas:** son proteínas relacionadas por homología con una identidad de secuencia >30%, estructura y función similares
- **Superfamilias proteicas:** proteínas o dominios que tienen baja identidad de secuencia, pero presentan aspectos estructurales y funcionales similares.



# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

- Recursos informáticos: Pfam → InterPro ([www.ebi.ac.uk/interpro](http://www.ebi.ac.uk/interpro))



The screenshot shows the InterPro website homepage. The header is blue with the InterPro logo and the text 'Classification of protein families'. Below the header is a navigation bar with links: Home, Search, Browse, Results, Release notes, Download, Help, and About. The main content area features a large graphic on the left with diagonal stripes and a red badge indicating 'InterPro 95.0' as of '29 June 2023'. To the right of the graphic is the title 'Classification of protein families' followed by a paragraph describing the service. Below this is a section titled 'Citing InterPro' with a reference to a 2022 publication in Nucleic Acids Research. At the bottom, a light blue banner contains a megaphone icon and text announcing that InterPro is the new home of Pfam, providing information about the shutdown of the Pfam website and the availability of a legacy version.

**InterPro** Classification of protein families

Home Search Browse Results Release notes Download Help About

**Classification of protein families**

InterPro provides functional analysis of proteins by classifying them into families and predicting domains and important sites. To classify proteins in this way, InterPro uses predictive models, known as signatures, provided by several different databases (referred to as member databases) that make up the InterPro consortium. We combine protein signatures from these member databases into a single searchable resource, capitalising on their individual strengths to produce a powerful integrated database and diagnostic tool.

▼ Citing InterPro

If you find InterPro useful, please cite the reference that describes this work:

Paysan-Lafosse T, Blum M, Chuguransky S, Grego T, Pinto BL, Salazar GA, Bileschi ML, Bork P, Bridge A, Colwell L, Gough J, Haft DH, Letunić I, Marchler-Bauer A, Mi H, Natale DA, Orengo CA, Pandurangan AP, Rivoire C, Sigrist CJA, Sillitoe I, Thanki N, Thomas PD, Tosatto SCE, Wu CH, Bateman A. *InterPro in 2022. Nucleic Acids Research*, Nov 2022, (doi: 10.1093/nar/gkac993)

**InterPro is the new home of Pfam**


The Pfam website ([pfam.xfam.org](http://pfam.xfam.org)) was shut down on October 5th, but InterPro offers the same functionality and data. A legacy version of Pfam is available at <https://pfam-legacy.xfam.org/> but will not receive any updates and will be decommissioned in Spring 2023.



### 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

- Recursos informáticos: Pfam → InterPro


Classification of protein families

[Home](#)
[Search](#)
[Browse](#)
[Results](#)
[Release notes](#)
[Download](#)
[Help](#)
[About](#)

Status

finished

Expires

Wed Aug 30 2023

### Protein family membership

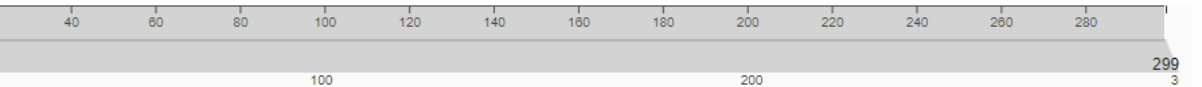
Two pore domain potassium channel (IPR003280)

Two pore domain potassium channel, TRAAK (IPR008074)

Entry matches to this protein

Options

Export



Family

2por... TRAAK...

2pore... TRAAKC...

2por... TRAA...

2por... TRAAK...

2pore\_dom\_K\_chnl

POTASSIUM CHANNEL, SUBFAMILY K

2POREKCHANNEL

2...

Domain

K\_chnl\_dom

Ion\_trans\_2

K\_chnl\_dom

Ion\_trans\_2

Unintegrated

Voltage-gated ...

Voltage-gated potassium chann...

Voltage-gated potassium channels

Other Features

Transm...

Transm...

Transm...

Transm...

Transm...

Transme...

IPR008074 PR01691

IPR003280 PTHR11003 PR01333

IPR013099 PF07885

G3DSA:1.10.287.70

SSF81324

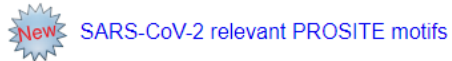
TRANSMEMBRANE

# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

- Recursos informáticos: **PROSITE** ([prosite.expasy.org](https://prosite.expasy.org))

### Database of protein domains, families and functional sites



PROSITE consists of documentation entries describing protein domains, families and functional sites as well as associated patterns and profiles to identify them [[More...](#) / [References](#) / [Commercial users](#)].

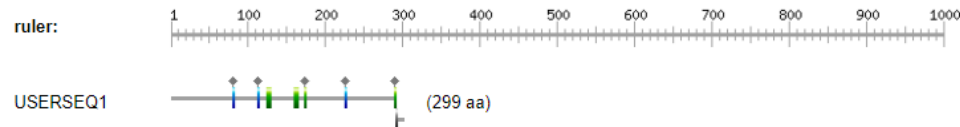
PROSITE is complemented by [ProRule](#), a collection of rules based on profiles and patterns, which increases the discriminatory power of profiles and patterns by providing additional information about functionally and/or structurally critical amino acids [[More...](#)].

#### Legend:

disulfide bridge    active site    other 'ranges'    other sites

Please note that the graphical representations of domains displayed hereafter are for illustrative purposes only, and that their colors and shapes are not intended to indicate homology or shared function. For more information about how these graphical representations are constructed, go to <https://prosite.expasy.org/mydomains/>.

hits by patterns with a high probability of occurrence or by user-defined patterns: [8 hits (by 4 distinct patterns) on 1 sequence]



PS00006 CK2_PHOSPHO_SITE Casein kinase II phosphorylation site :			
80 - 83:	SdqE		
Predicted feature:			
MOD_RES	80	Phosphoserine	[condition: S]
112 - 115:	SawD		
Predicted feature:			
MOD_RES	112	Phosphoserine	[condition: S]
224 - 227:	Sk1E		
Predicted feature:			
MOD_RES	224	Phosphoserine	[condition: S]
PS00008 MYRISTYL N-myristoylation site :			
124 - 129:	GTiITT		
158 - 163:	GILLAG		
PS00005 PKC_PHOSPHO_SITE Protein kinase C phosphorylation site :			
171 - 173:	S1R		
Predicted feature:			
MOD_RES	171	Phosphoserine	[condition: S]



# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

- Recursos informáticos: SCOP (<https://scop.mrc-lmb.cam.ac.uk>)

### SCOP 2

[Learn More](#)

#### SCOP: Structural Classification of Proteins

Nearly all proteins have structural similarities with other proteins and, in some of these cases, share a common evolutionary origin. The SCOP database, created by manual inspection and abetted by a battery of automated methods, aims to provide a detailed and comprehensive description of the structural and evolutionary relationships between all proteins whose structure is known. As such, it provides a broad survey of all known protein folds, detailed information about the close relatives of any particular protein, and a framework for future research and classification.

Latest update on **2022-06-29** includes **72,544** non-redundant domains representing **861,631** protein structures. Folds, superfamilies and families statistics [here](#).

[Keyword and ID search](#)[Sequence search](#)

Enter free text, SCOP ID, PDB ID or UniProt ID

Go

#### Browse by structural class

- [All alpha proteins](#)
- [All beta proteins](#)
- [Alpha and beta proteins\(a/b\)](#)
- [Alpha and beta proteins\(a+b\)](#)
- [Small proteins](#)

#### Browse by protein type

- [Globular proteins](#)
- [Membrane proteins](#)
- [Fibrous proteins](#)
- [Non-globular/Intrinsically unstructured proteins](#)

# 3.1. Aspectos estructurales de las proteínas

## Estructura de las proteínas:

- Recursos informáticos: SCOP (<https://scop.mrc-lmb.cam.ac.uk>)

**DOMAIN**  
**1P7B A:59-151**

Inward rectifier potassium channel

Species *Burkholderia pseudomallei*

Show ancestry ☒

```
graph BT; A["class 1000000<br/>All alpha proteins"] <--> B["fold 2000019<br/>Voltage-gated potassium channels"]; B <--> C["superfamily 3000023<br/>Voltage-gated potassium channels"]; C <--> D["family 4000034<br/>Voltage-gated potassium channels"]; D <--> E["domain 8003429"];
```

**Representative sequence**   Other domains for this sequence   External links

UniProtP83698  
This domain

MNVDFSPHS SDSFAQAAPF ARKPPRGRR IWSGTREVA YGMPASVWRD LYYWALKVSW PVFFASLAAL FVNNTLFAL LYQLGDAPIA NQSPPGFVGA FFFSVETLAT VGYGDMHPQT VYAHAIATLE IFVGMGIAL STGLVFARFA RPRAKIMFAR HAIVRFNGR MTLMVRAANA RQNVIAEARA KMRLMRREHS SEGYSIMKIH DLKLVNNEHP IFLLGWNMMH VIDESSPLFG ETPESLAEGR AMLLVMIEGS DETTAQVMQA RHAWEHDDIR WHHRIVDLMS DVDGMTHIDY TRFNDTEPVE PFGAAPDAQA FAKPFGEDA RFV

Domain only  
Domain in chain  
Domain in PDB

SCOP2 2021 / supported by the UK Medical Research council (MRC)  
Structural Classification of Proteins by Antonina Andreeva, Eugene Kulesha, Julian Gough, Andrey Morzin is licensed under [CC BY 4.0](#)

Build 1.0.6

# Temario - Contenidos

## Tema 3. Proteómica estructural

3.1. Aspectos estructurales de las proteínas: niveles de organización

3.2. Métodos de caracterización estructural en proteómica

3.3. Servidores y bases de datos en proteómica estructural

3.4. Bioinformática estructural

## 3.2. Métodos de caracterización estructural

### Determinación estructural experimental:

#### ○ Cristalografía de rayos X (X-ray)

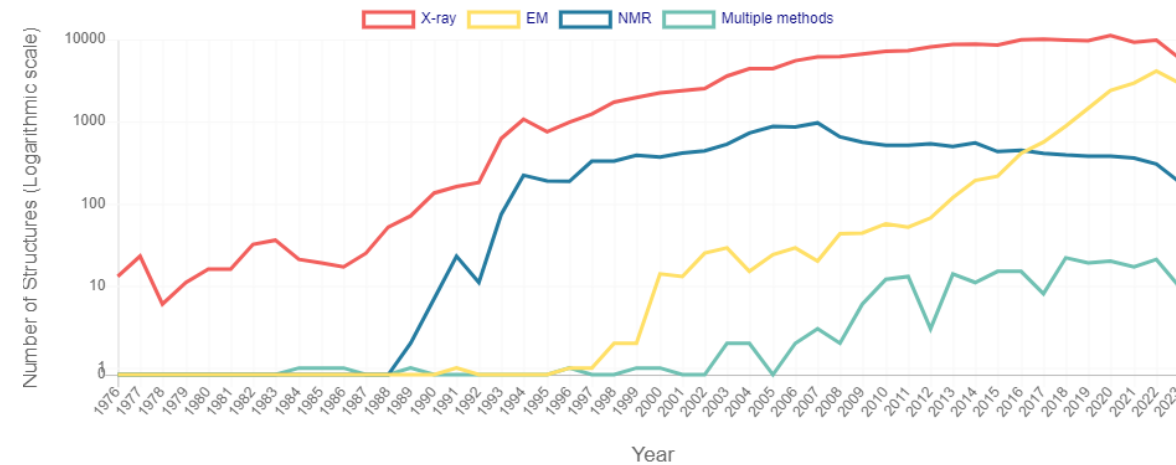
- Difracción de rayos X por sólidos cristalinos
- Tipo y posición de átomos
- Sin límite de tamaño
- Mejores resoluciones
- Requisito: cristalizar, cristales de calidad

#### ○ Resonancia magnética nuclear (NMR)

- Un campo magnético externo hace que ciertos núcleos absorban radiofrecuencias selectivas. La energía absorbida induce una transición en el espín nuclear, observándose en el espectro RMN.
- **Ensamblados conformacionales**
- Limitaciones de tamaño (depende de potencia del campo magnético)

#### ○ Crio-electromicroscopía (Cryo-EM)

- Estudio a temperatura criogénica evitando artefactos
- Tomografía crioeléctronica para reconstruir en 3D imágenes 2D anguladas.
- Resolución similar X-ray
- Número de estructuras resueltas aumentando



## 3.2. Métodos de caracterización estructural

### Determinación estructural experimental:

- Archivos PDB (ProteinDataBank)

```
HEADER    TRANSPORT PROTEIN                22-JAN-19   6NR4
TITLE     CRYO-EM STRUCTURE OF THE TRPM8 ION CHANNEL WITH LOW OCCUPANCY ICILIN,
TITLE     2 PI(4,5)P2, AND CALCIUM
COMPND    MOL_ID: 1;
COMPND    2 MOLECULE: TRANSIENT RECEPTOR POTENTIAL CATION CHANNEL SUBFAMILY M
COMPND    3 MEMBER 8;
COMPND    4 CHAIN: A, B, C, D;
COMPND    5 ENGINEERED: YES;
COMPND    6 MUTATION: YES
SOURCE    MOL_ID: 1;
SOURCE    2 ORGANISM_SCIENTIFIC: FICEDULA ALBICOLLIS;
SOURCE    3 ORGANISM_COMMON: COLLARED FLYCATCHER;
SOURCE    4 ORGANISM_TAXID: 59894;
SOURCE    5 GENE: TRPM8;
SOURCE    6 EXPRESSION_SYSTEM: HOMO SAPIENS;
SOURCE    7 EXPRESSION_SYSTEM_TAXID: 9606
KEYWDS    ION CHANNEL, TRP CHANNEL, TRPM CHANNEL, TRPM8 CHANNEL, COLD SENSING,
KEYWDS    2 LIPID SENSING, MENTHOL, ICILIN, WS-12, PI(4, 5)P2, CALCIUM-PERMEABLE
KEYWDS    3 CHANNEL, COOLING AGENT, TRANSPORT PROTEIN
EXPDTA    ELECTRON MICROSCOPY
AUTHOR    Y.YIN,S.C.LE,A.L.HSU,M.J.BORGNIA,H.YANG,S.-Y.LEE
REVDAT    4   18-DEC-19  6NR4   1   SCALE
REVDAT    3   13-MAR-19  6NR4   1   JRNL
REVDAT    2   27-FEB-19  6NR4   1   KEYWDS
REVDAT    1   20-FEB-19  6NR4   0
JRNL      AUTH    Y.YIN,S.C.LE,A.L.HSU,M.J.BORGNIA,H.YANG,S.-Y.LEE
JRNL      TITL    STRUCTURAL BASIS OF COOLING AGENT AND LIPID SENSING BY THE
JRNL      TITL    2 COLD-ACTIVATED TRPM8 CHANNEL.
JRNL      REF     SCIENCE                               V. 363       2019
JRNL      REFN    ESSN 1095-9203
JRNL      PMID    30733385
JRNL      DOI     10.1126/SCIENCE.AAV9334
```

```
REMARK 247 ELECTRON MICROSCOPY
REMARK 247 THE COORDINATES IN THIS ENTRY WERE GENERATED FROM ELECTRON
REMARK 247 MICROSCOPY DATA. PROTEIN DATA BANK CONVENTIONS REQUIRE
REMARK 247 THAT CRYST1 AND SCALE RECORDS BE INCLUDED, BUT THE VALUES
REMARK 247 ON THESE RECORDS ARE MEANINGLESS EXCEPT FOR THE CALCULATION
REMARK 247 OF THE STRUCTURE FACTORS.
REMARK 300
REMARK 300 BIOMOLECULE: 1
REMARK 300 SEE REMARK 350 FOR THE AUTHOR PROVIDED AND/OR PROGRAM
REMARK 300 GENERATED ASSEMBLY INFORMATION FOR THE STRUCTURE IN
REMARK 300 THIS ENTRY. THE REMARK MAY ALSO PROVIDE INFORMATION ON
REMARK 300 BURIED SURFACE AREA.
REMARK 350
REMARK 350 COORDINATES FOR A COMPLETE MULTIMER REPRESENTING THE KNOWN
REMARK 350 BIOLOGICALLY SIGNIFICANT OLIGOMERIZATION STATE OF THE
REMARK 350 MOLECULE CAN BE GENERATED BY APPLYING BIOMT TRANSFORMATIONS
REMARK 350 GIVEN BELOW. BOTH NON-CRYSTALLOGRAPHIC AND
REMARK 350 CRYSTALLOGRAPHIC OPERATIONS ARE GIVEN.
REMARK 350
REMARK 350 BIOMOLECULE: 1
REMARK 350 AUTHOR DETERMINED BIOLOGICAL UNIT: TETRAMERIC
REMARK 350 APPLY THE FOLLOWING TO CHAINS: A, B, C, D
REMARK 350 BIOMT1   1   1.000000   0.000000   0.000000   0.00000
REMARK 350 BIOMT2   1   0.000000   1.000000   0.000000   0.00000
REMARK 350 BIOMT3   1   0.000000   0.000000   1.000000   0.00000
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ATOM 5129 ND2 ASN A 972      153.460 134.596 175.301  1.00 44.88      N
ATOM 5130 N   LEU A 973      148.369 134.918 173.838  1.00 48.30      N
ATOM 5131 C   LEU A 973      146.951 134.575 173.773  1.00 48.30      C
ATOM 5132 C   LEU A 973      146.317 135.117 172.500  1.00 48.30      C
ATOM 5133 O   LEU A 973      145.555 134.418 171.822  1.00 48.30      O
ATOM 5134 CB  LEU A 973      146.231 135.124 175.011  1.00 48.30      C
ATOM 5135 N   LEU A 974      146.641 136.359 172.146  1.00 49.12      N
ATOM 5136 CA  LEU A 974      145.985 136.950 170.990  1.00 49.12      C
ATOM 5137 C   LEU A 974      146.613 136.486 169.683  1.00 49.12      C
ATOM 5138 O   LEU A 974      145.979 136.584 168.627  1.00 49.12      O
ATOM 5139 CB  LEU A 974      145.997 138.465 171.121  1.00 49.12      C
```

## 3.2. Métodos de caracterización estructural

**Determinación estructural a escala proteómica:** mejora en tecnología y automatización

- PSI – Protein Structure Initiative – hasta año 2015
- SGC – Structural Genomics Consortium – 1500 proteínas resueltas

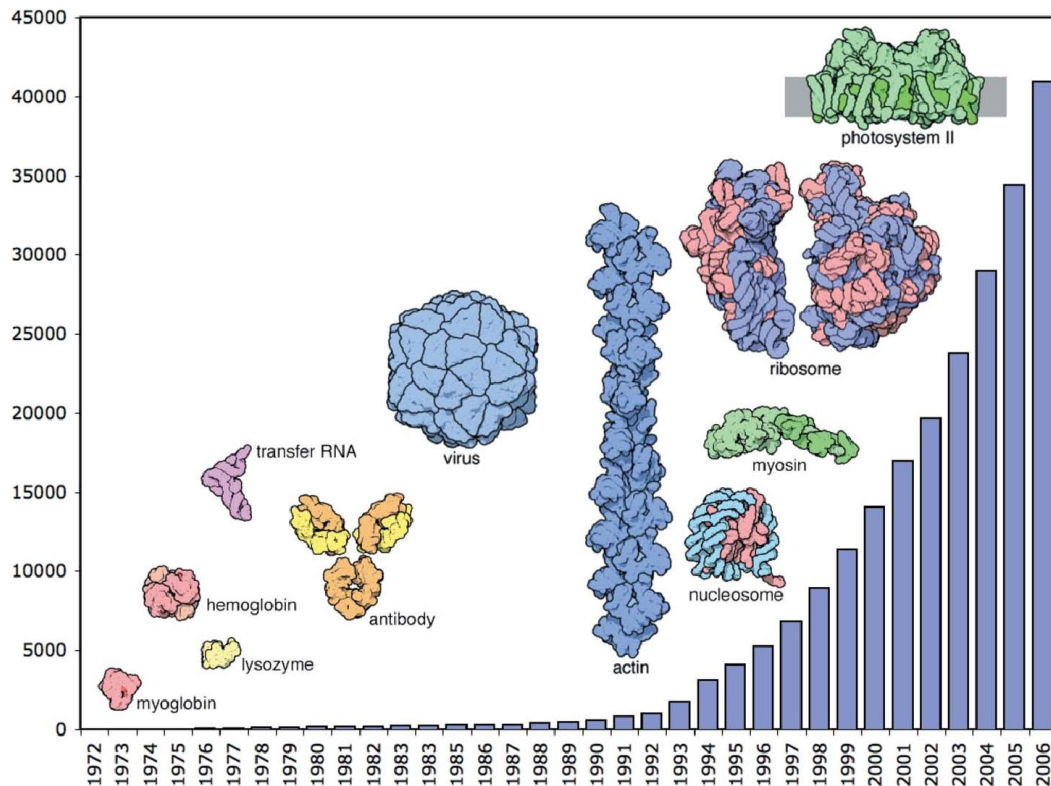


Figure 1

**The Structural Genomics Consortium (SGC) is a global public-private partnership dedicated to open science.**

**2003**

Established as a charity in the UK and co-founded by global pharmaceutical organizations, government agencies and international foundations

**\$400M+**

In R&D funding to support early-stage projects since inception

**8 Industry Partners**



**6 Research Sites**



**Major**

**Funding Supporters Include**



**330+**

**Partnerships**

**25+**

**Publications with industry partners each year**

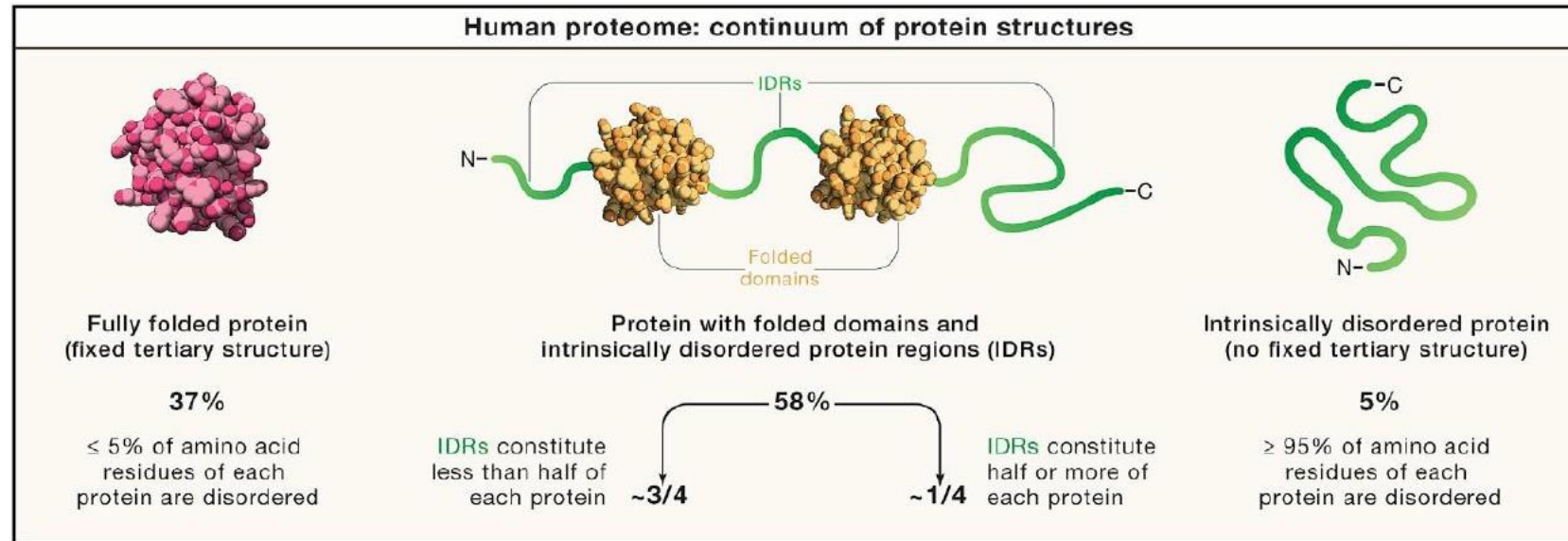


## 3.2. Métodos de caracterización estructural

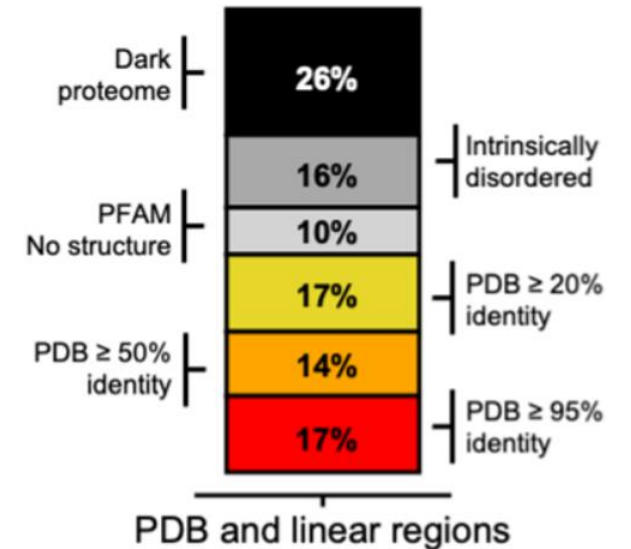
### El proteoma estructural humano:

Se estima que existen unas **20.000 proteínas humanas** (no redundantes)

En los últimos **10 años**, los proyectos de proteómica han identificado unas **18.000 proteínas** (!!)



*Tsang et al. 2020 Cell 183, 1742*



# Temario - Contenidos

## Tema 3. Proteómica estructural

3.1. Aspectos estructurales de las proteínas: niveles de organización

3.2. Métodos de caracterización estructural en proteómica

3.3. Servidores y bases de datos en proteómica estructural

3.4. Bioinformática estructural



# 3.3. Servidores y bases de datos en proteómica estructural

- Protein Data Bank (PDB)
- CATH ([www.cathdb.info](http://www.cathdb.info))

**CATH / Gene3D v4.3**  
151 million protein domains classified into 5,841 superfamilies

Search by keywords, PDB code, GO term, etc **Search**

Core classification files for the latest version of CATH-Plus (v4.3) are [now available to download](#). [Daily updates](#) of our very latest classifications are also available.

**3D Structure**  
Find out what 3D structure your protein adopts  
[Find out more](#) [Go](#)

**Protein Evolution**  
Learn about a particular protein family and how it evolved  
[Find out more](#)

**Protein Function**  
Investigate the function of your protein  
[Find out more](#) [Go](#)

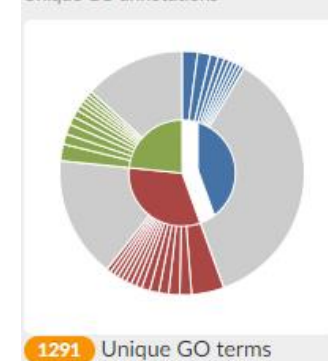
**Conserved Sites**  
Look at protein sites that are highly conserved and implicated in function  
[Find out more](#) [Go](#)

**Download Data**  
Download data files and query CATH via webservice  
[Go](#)

**SUPERFAMILY LINKS**  
[Summary](#)  
**Superfamily Superposition**  
[Classification / Domains](#)  
[Functional Families](#)  
[Structural Neighbourhood](#)

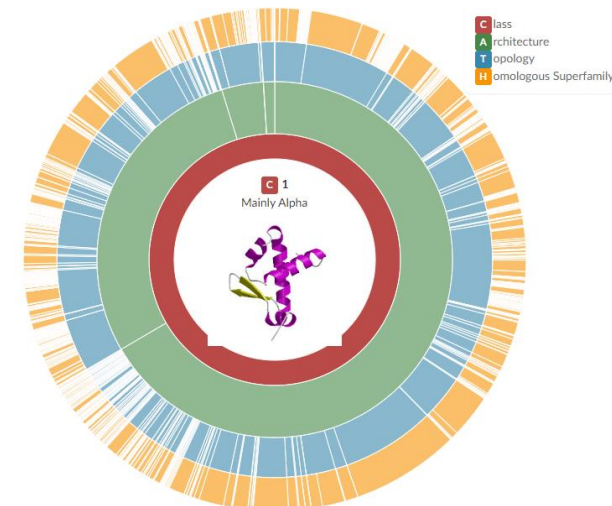
ID	Function Family (FunFam) Name	Total Sequences	Enzyme?	Structure?	Structural Representative	PDB Sites?	Alignment Diversity (0-100)
1	<a href="#">Sodium channel protein</a>	2092			-	-	84.7
2	<a href="#">Potassium voltage-gated channel subfamily a member</a>	1878		<b>3D</b>	<a href="#">4jtdH03</a>	-	96.2

Molecular function: protein binding  
Biological process: potassium ion transport  
Cellular component: plasma membrane



## CATH Classification

Level	CATH Code	Description
	<b>1</b>	<a href="#">Mainly Alpha</a>
	<b>1.10</b>	<a href="#">Orthogonal Bundle</a>
	<b>1.10.287</b>	<a href="#">Helix Hairpins</a>
	<b>1.10.287.70</b>	



# Temario - Contenidos

## Tema 3. Proteómica estructural

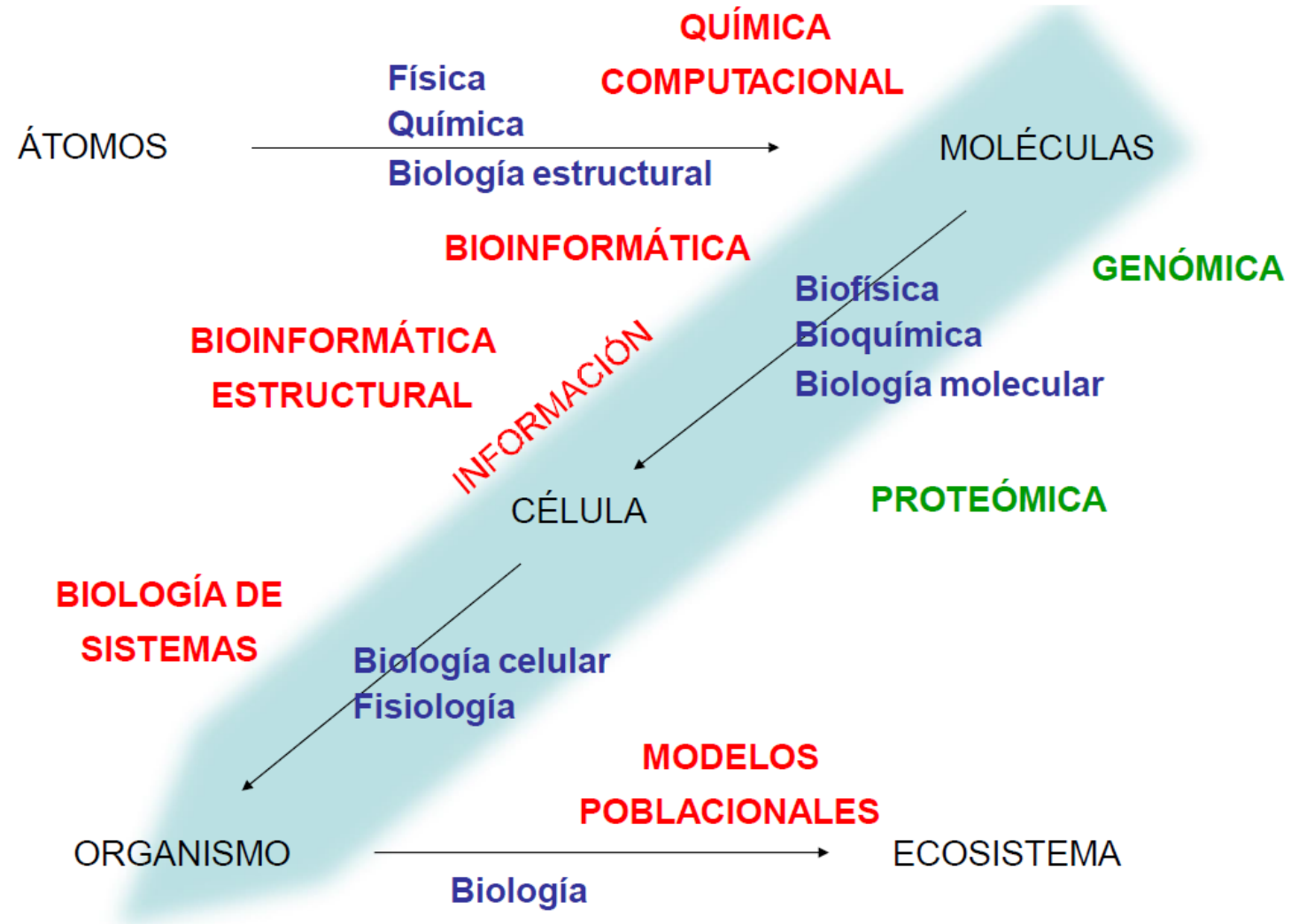
3.1. Aspectos estructurales de las proteínas: niveles de organización

3.2. Métodos de caracterización estructural en proteómica

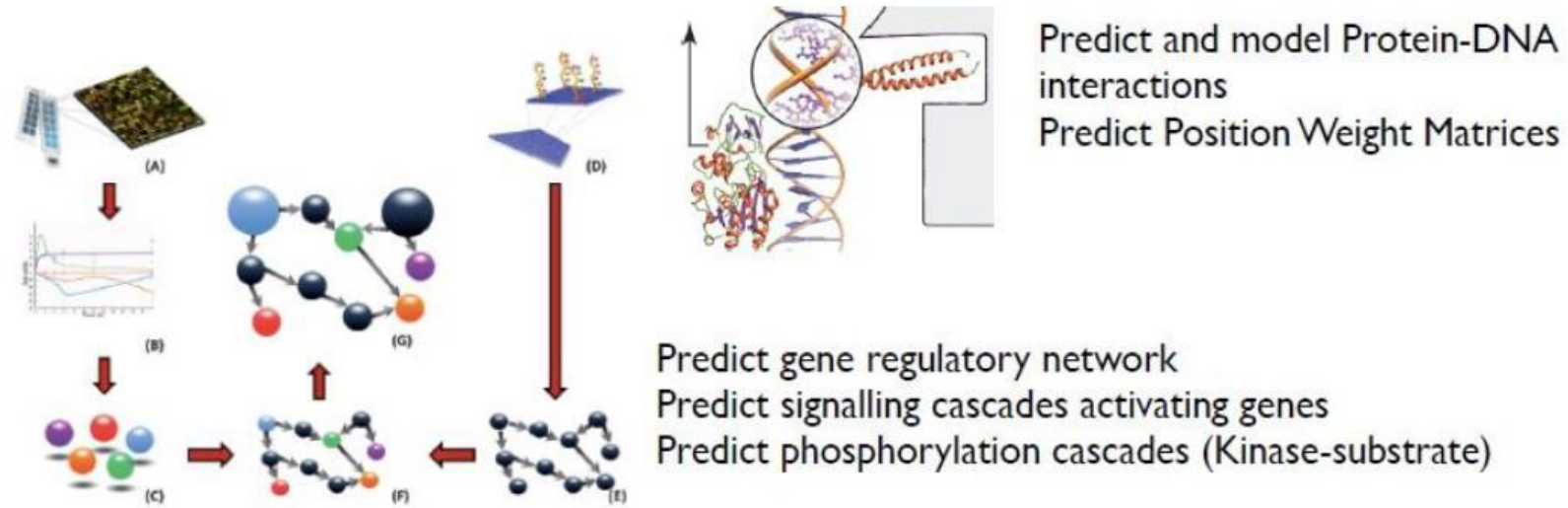
3.3. Servidores y bases de datos en proteómica estructural

3.4. Bioinformática estructural

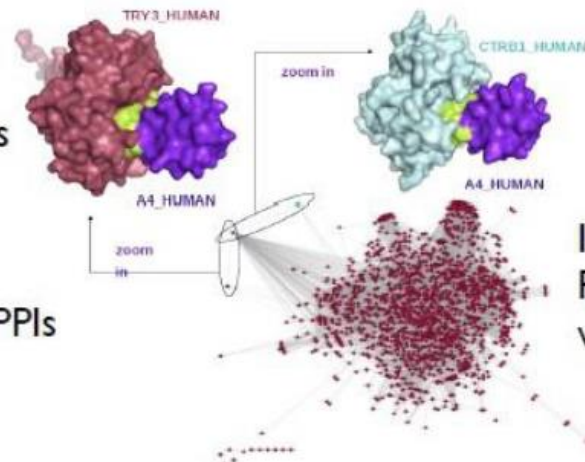
## 3.4. Bioinformática estructural



## 3.4. Bioinformática estructural



Predict the function of proteins  
Model the structure of proteins  
Predict protein-protein interactions  
Score reliability of PPIs  
Model the structure of PPIs  
Predict the strength of PPIs ( $K_a$ )  
Predict changes in the network of PPIs



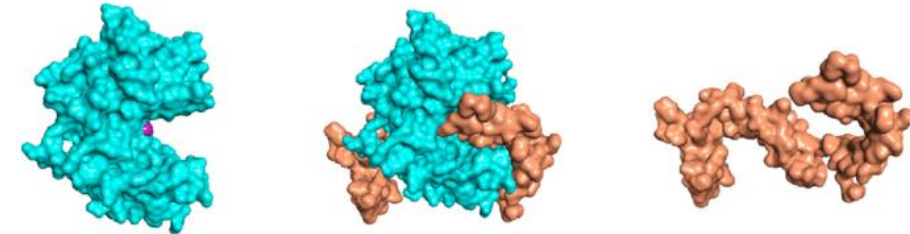
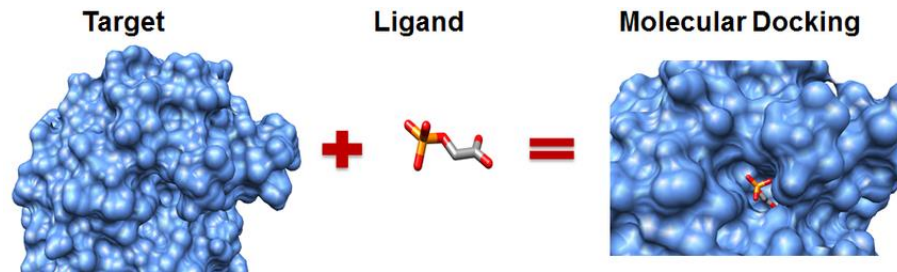
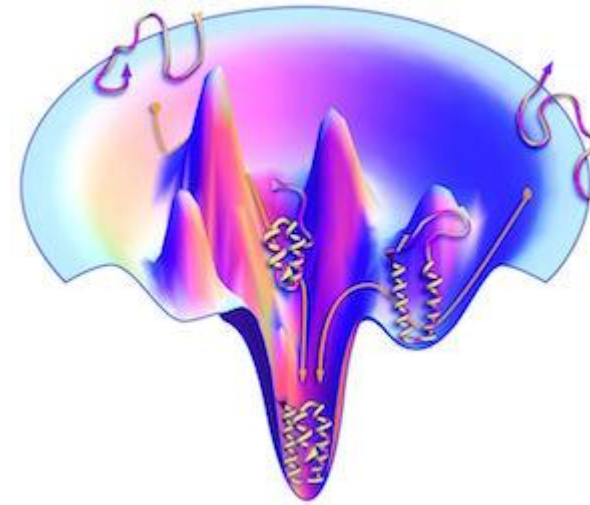
Integration of databases on PPIs  
Predict target genes associated with phenotypes



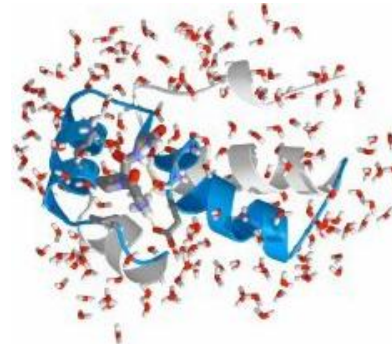
## 3.4. Bioinformática estructural

### Bioinformática estructural

- Plegamiento de proteínas (*folding*)
  - *Ab initio*
  - *Homology modelling*
- Acoplamiento molecular (*docking*)
  - Proteína-proteína
  - Proteína-péptido
  - Proteína-ligando químico
  - Proteína-ácido nucleico



- Dinámica molecular





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