

Máster Universitario en Bioinformática

Proteómica y Bioinformática Estructural

Curso académico 2024-2025



Universidad
Internacional
de Valencia

Dra. Magdalena Nikolaeva Koleva

magdalena.nikolaeva@professor.universidadviu.com

Sesión 3

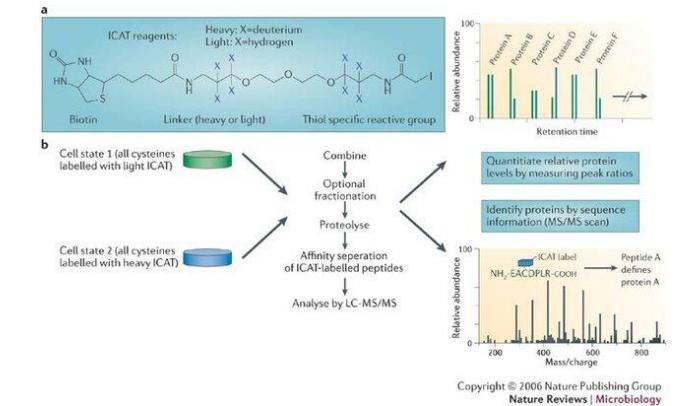
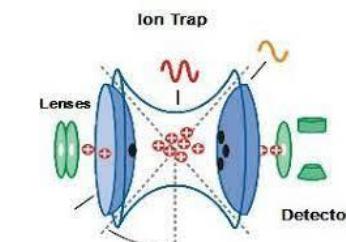
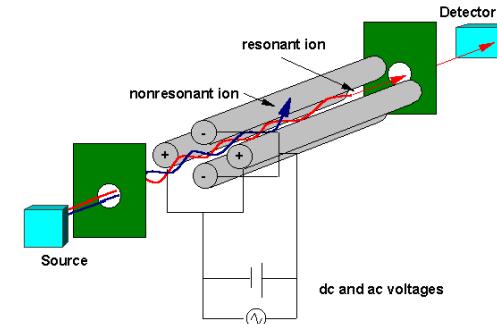
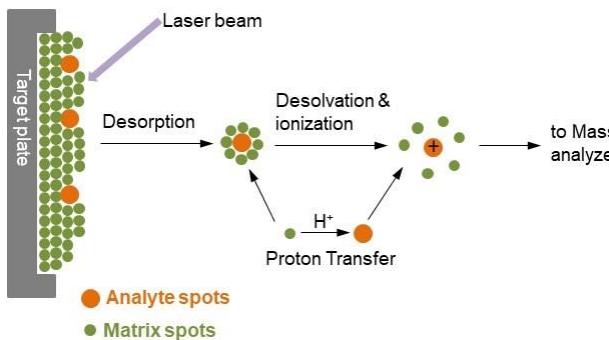
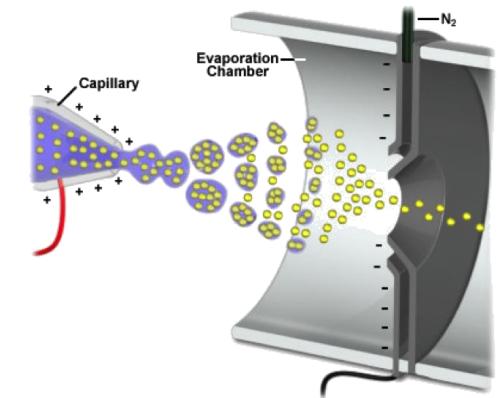
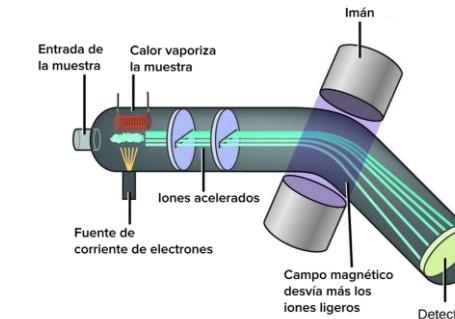
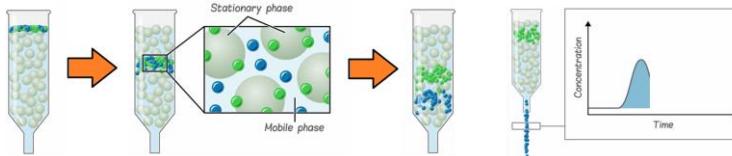
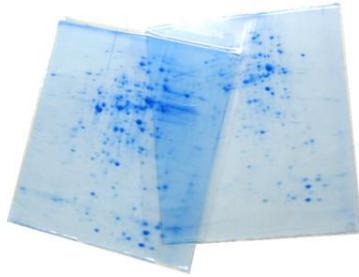
Proteómica estructural

The logo consists of the lowercase letters "viu" in white, centered within a solid orange rounded rectangle.

viu

Universidad
Internacional
de Valencia

¿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

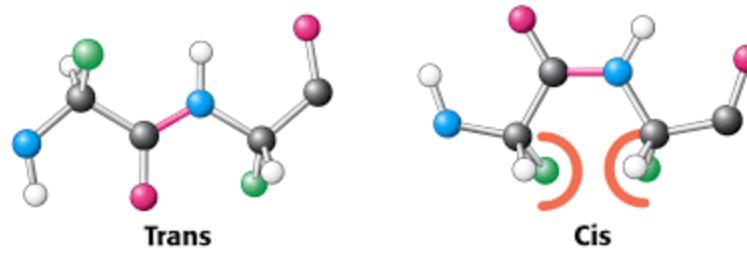
- 3.1. Aspectos estructurales de las proteínas: niveles de organización**
- 3.2. Métodos de caracterización estructural en proteómica
- 3.3. Servidores y bases de datos en proteómica estructural
- 3.4. Bioinformática estructural

3.1. Aspectos estructurales de las proteínas

Cadena polipeptídica:

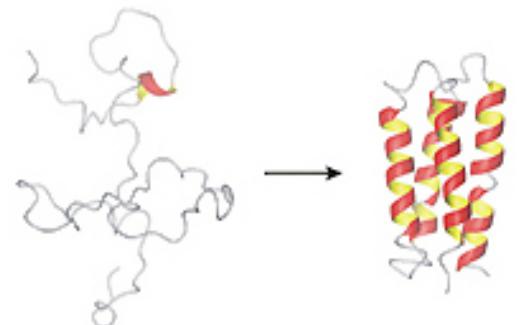
Presenta flexibilidad lo que le permite adoptar **diferentes conformaciones**, aunque con **ciertas restricciones**:

- Planaridad del enlace peptídico
- Choques estéricos de cadenas laterales



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

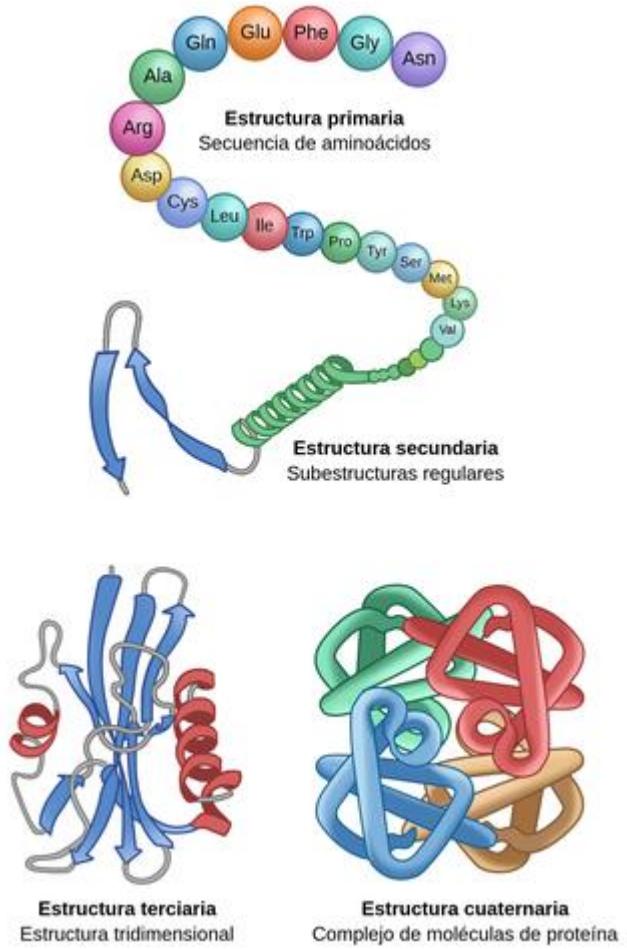
Desplegada:
Sin función



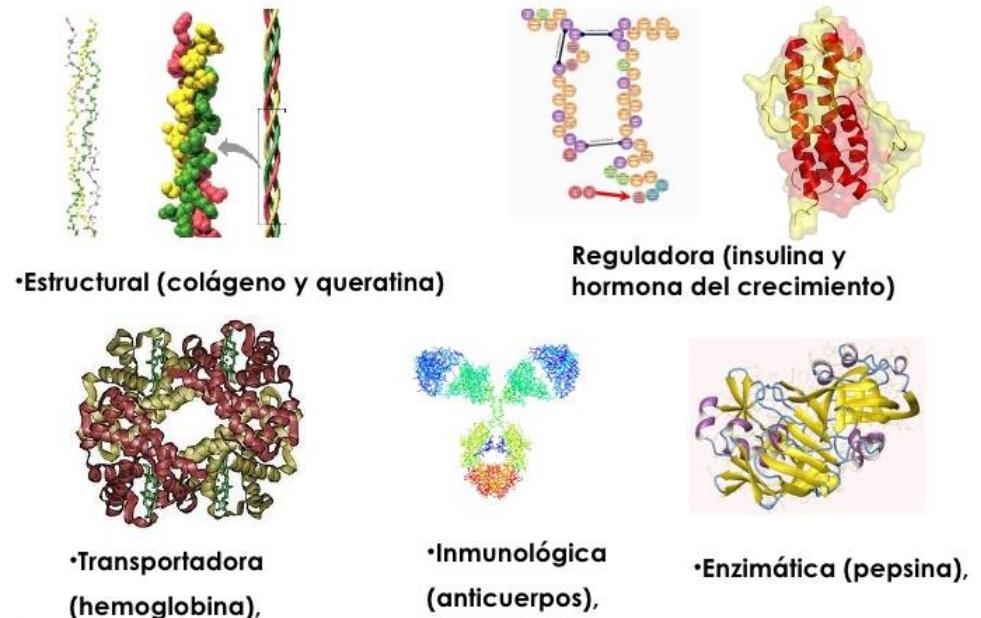
Plegada:
Con función

3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:



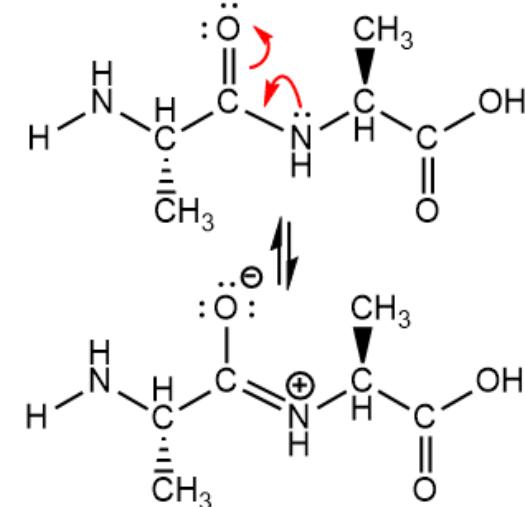
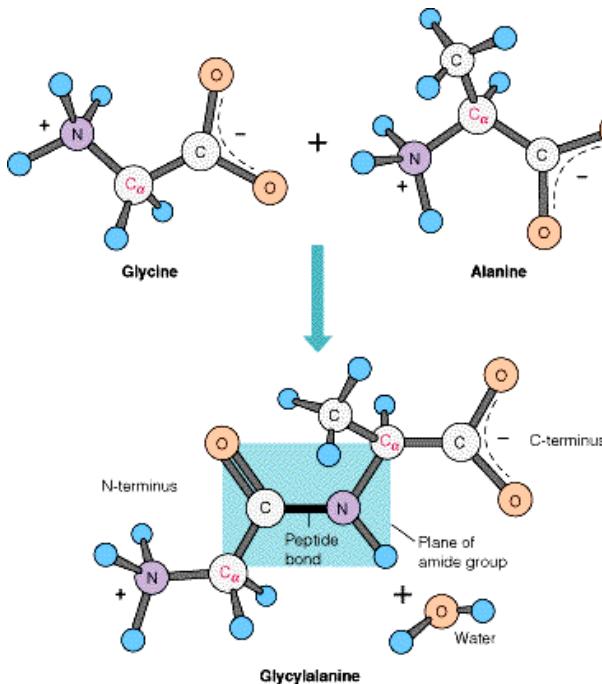
Plegamiento: estructura tridimensional única que determina la **función** específica de una proteína



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_α, psi – C_α-C)
 - Rotación libre
 - Determinante de conformaciones
 - Importancia cadena lateral (R) – restricciones de estructura química
- Ángulo enlace peptídico (omega – N-C)

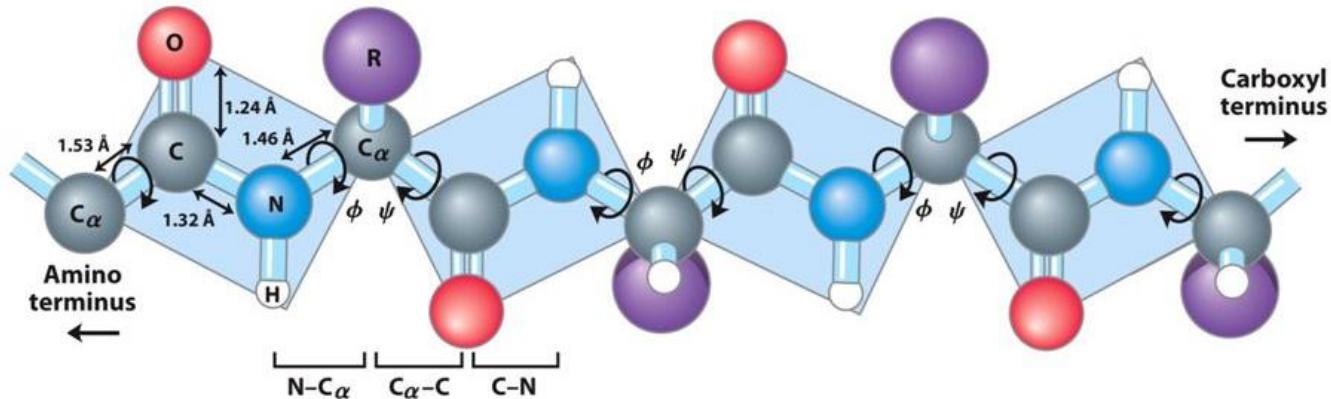


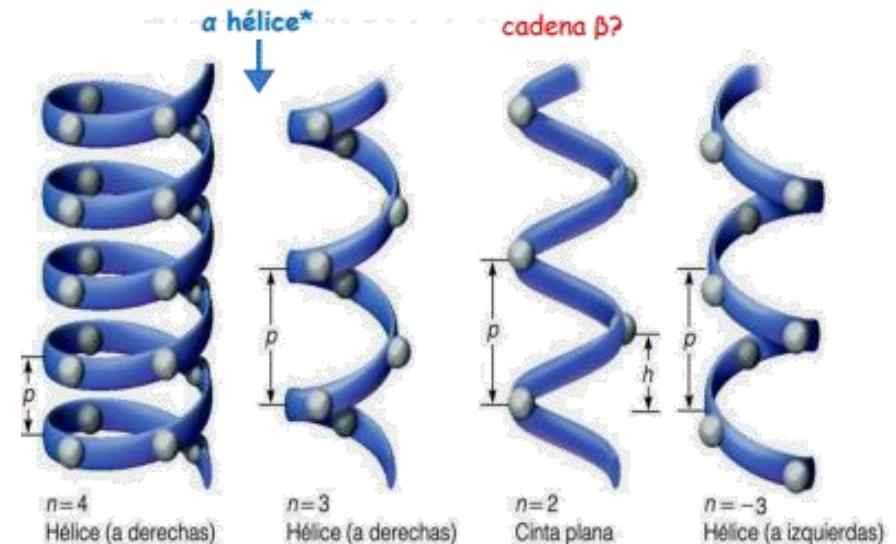
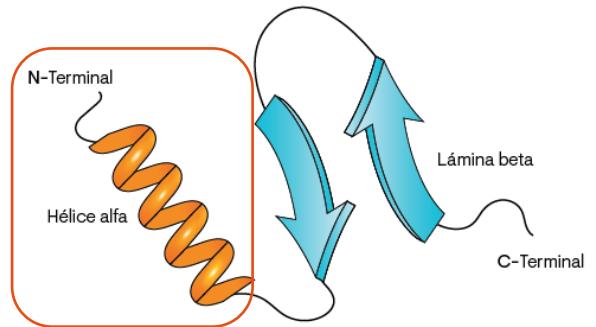
Figure 4-2b
Lehninger Principles of Biochemistry, Sixth Edition
© 2013 W. H. Freeman and Company

3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

○ Estructura secundaria:

- **Hélices:** p =paso de hélice, n =nº de residuos/vuelta
 - **hélice π :** $n=4.4$ residuos/vuelta, hueca por dentro, inestable
 - **α -hélice:** $n=3.6$ residuos/vuelta, $p=3.6 \times 0.15\text{nm}/\text{res}=0.56\text{nm}$
 - 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)

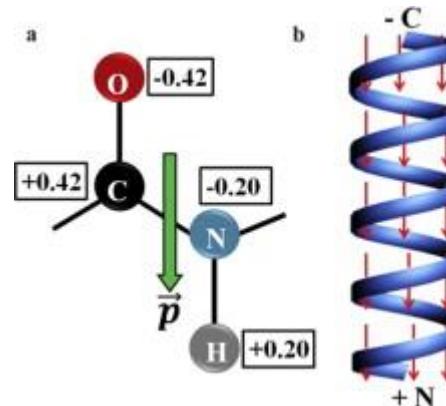
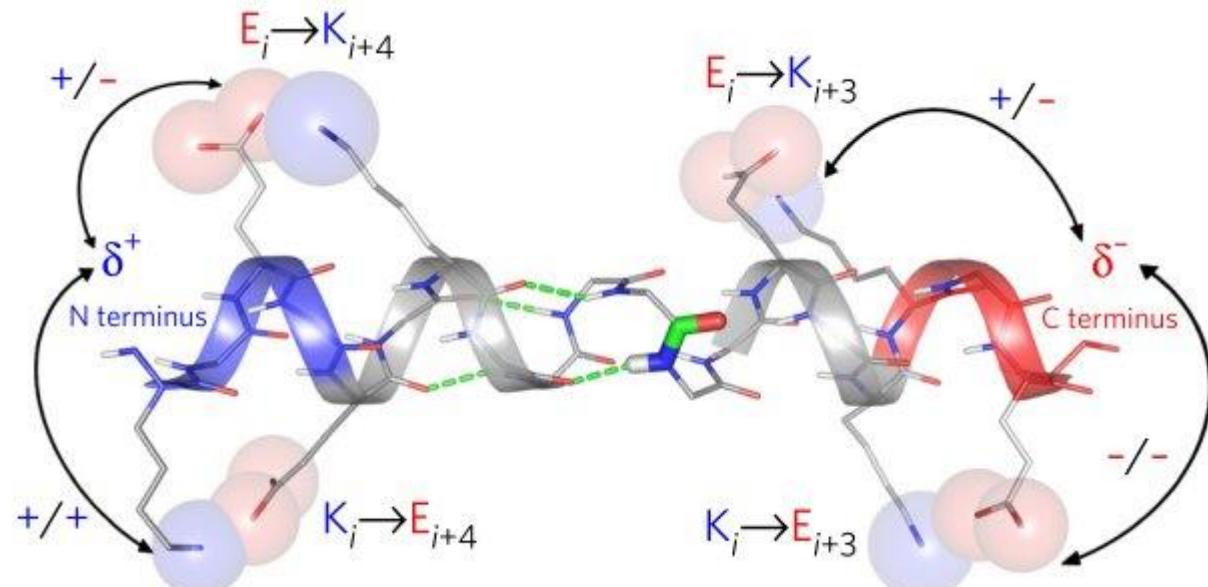
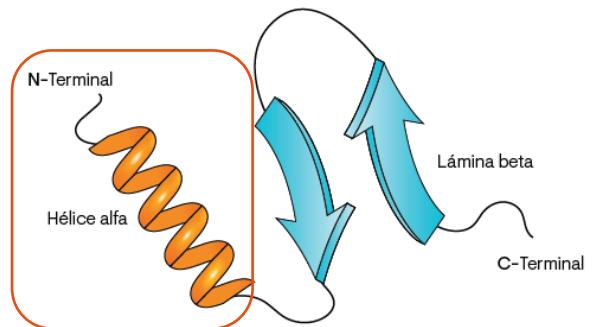


3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

○ Estructura secundaria:

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

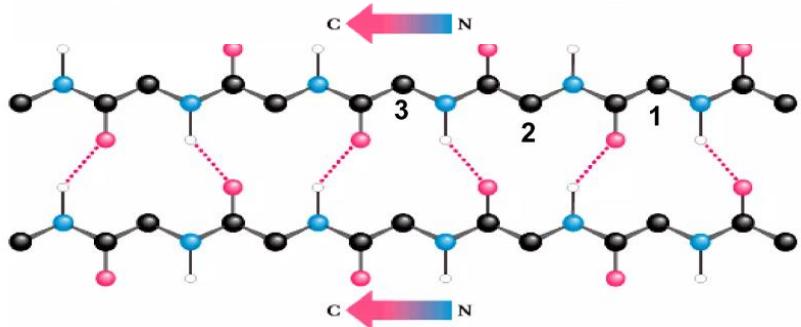
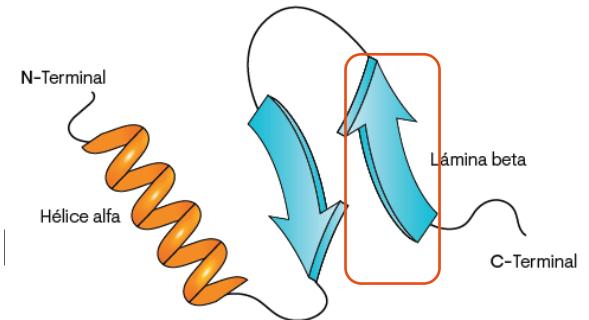


3.1. Aspectos estructurales de las proteínas

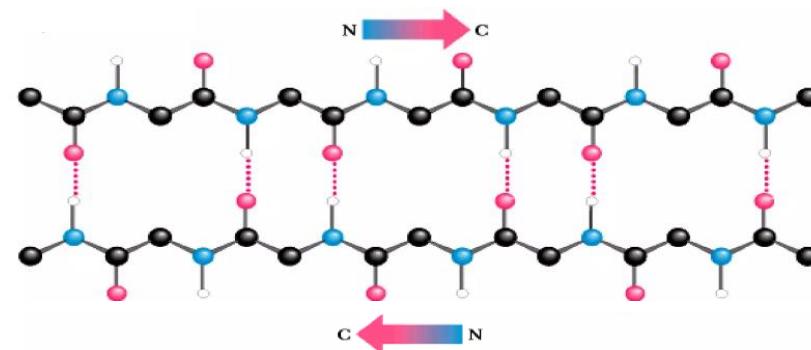
Estructura de las proteínas:

- Estructura secundaria:

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



Paralela

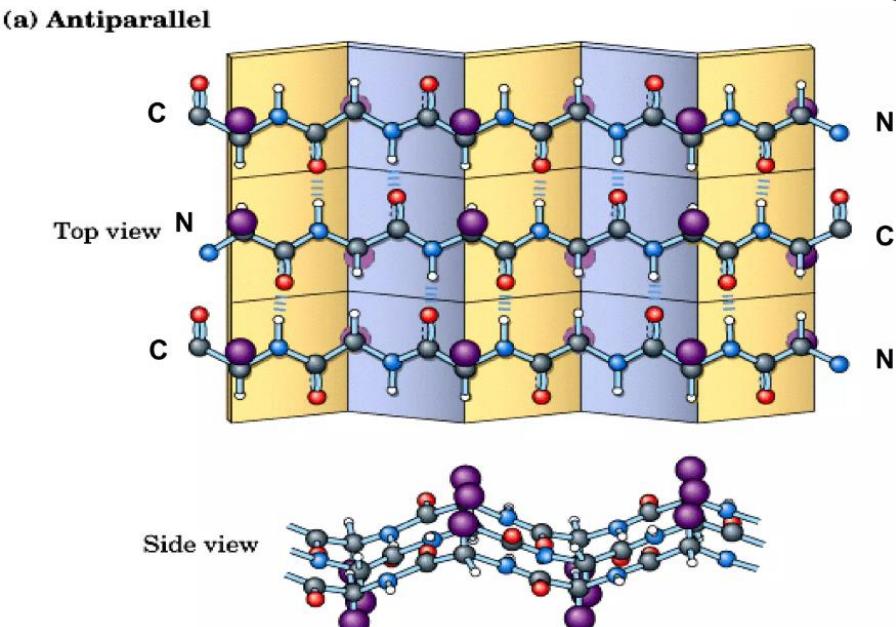
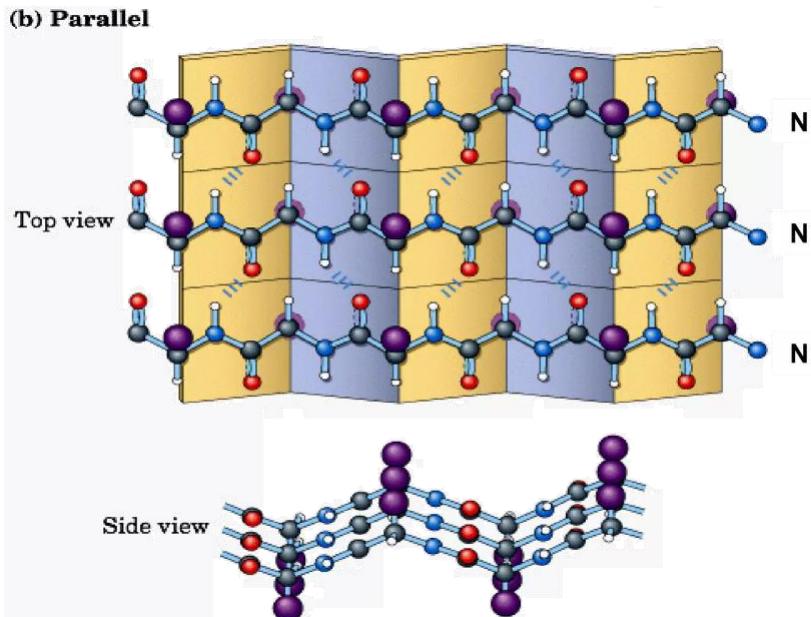
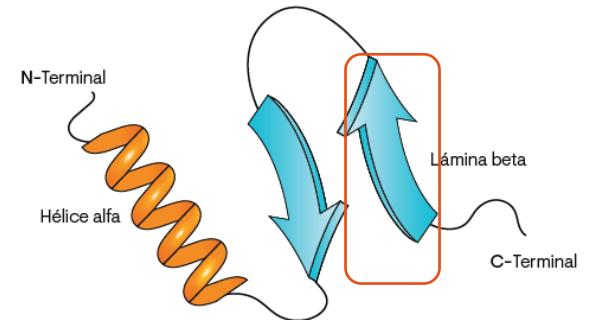


Antiparalela

3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

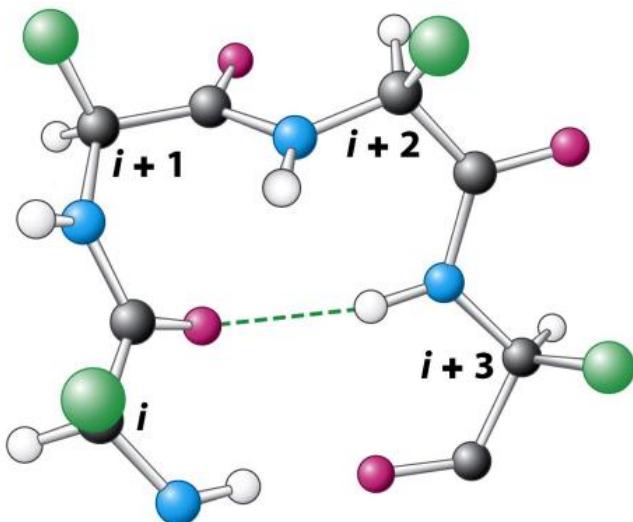
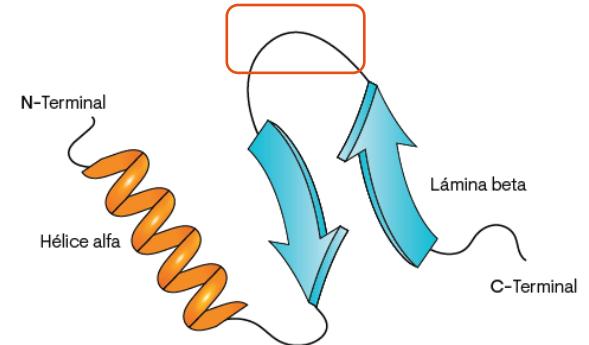
- Estructura secundaria:
 - Láminas- β - Hojas- β



3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

- Estructura secundaria:
 - **Giros- β :** 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

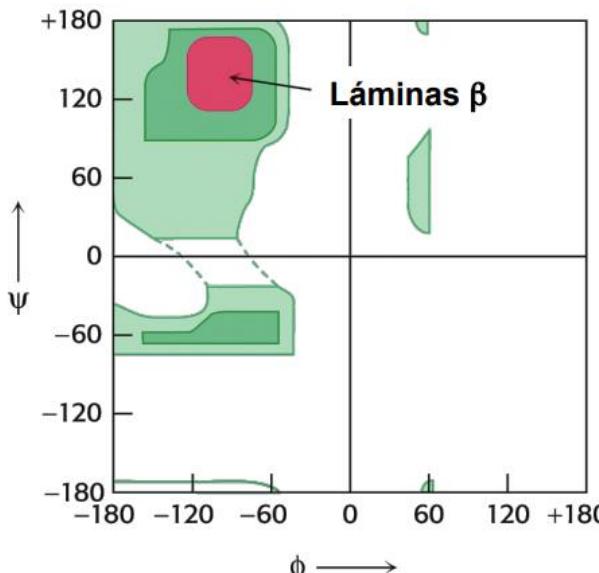
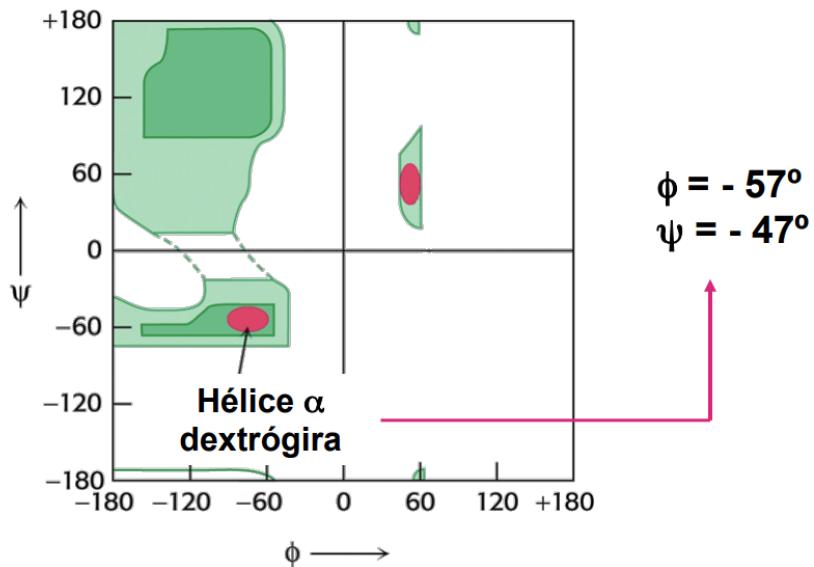
Estructura de las proteínas:

- Estructura secundaria:

- **Diagrama de Ramachandran:**

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

Identifica estructuras mal resueltas.



Paralela

$$\begin{aligned}\psi &= +113^\circ \\ \phi &= -119^\circ\end{aligned}$$

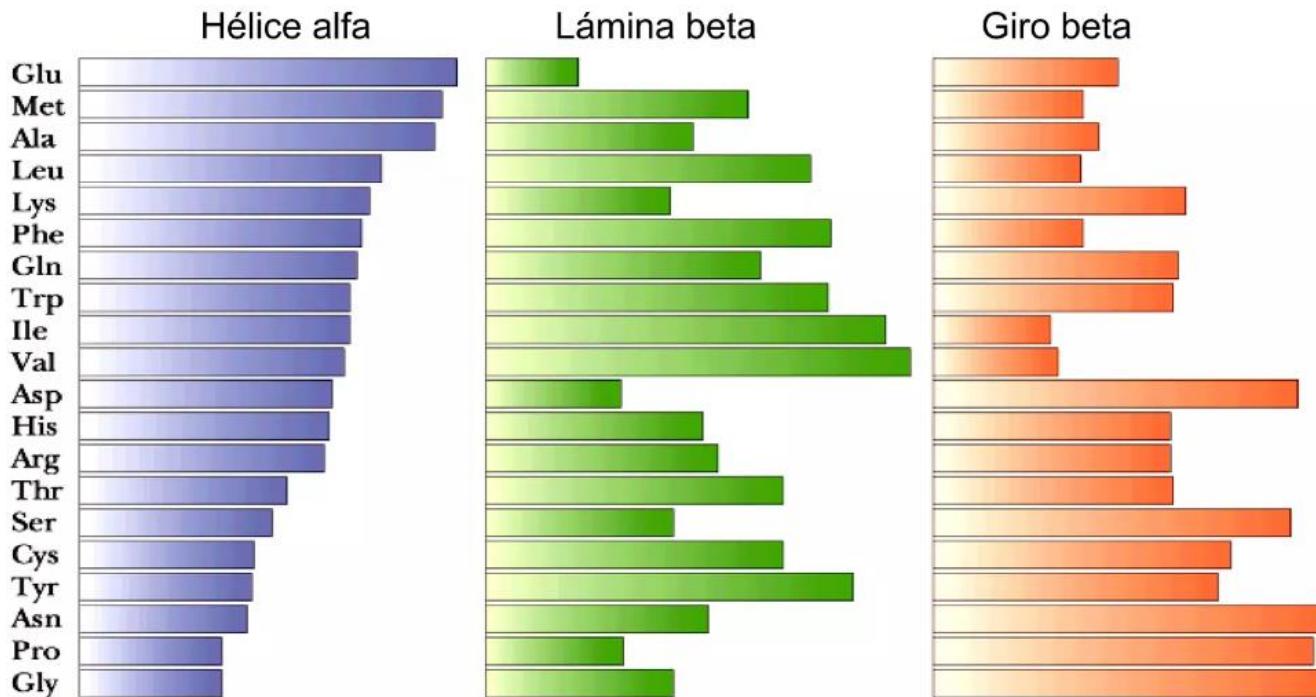
Antiparalela

$$\begin{aligned}\psi &= +135^\circ \\ \phi &= -139^\circ\end{aligned}$$

3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

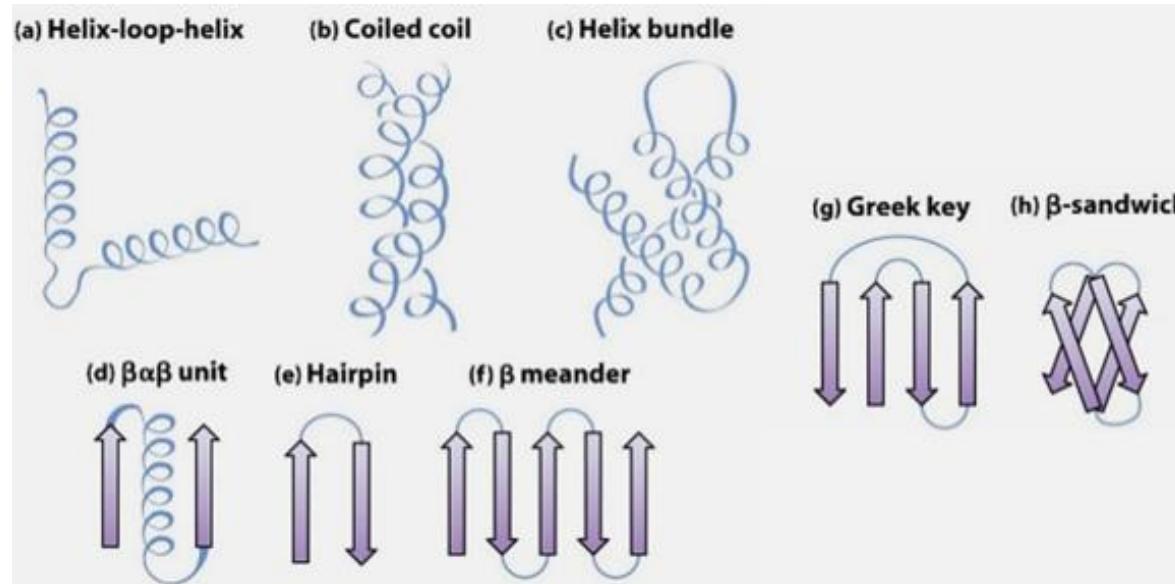
- Estructura secundaria:
 - Frecuencia relativa de aparición de aminoácidos en estructuras secundarias:



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

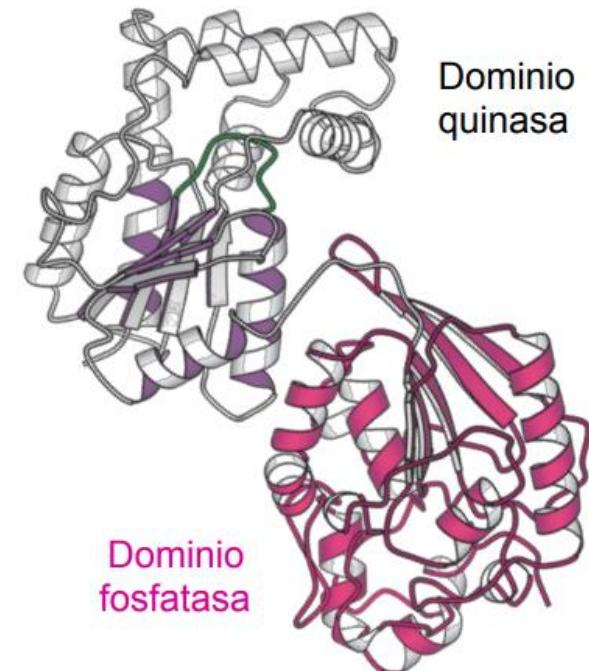


3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

○ Estructura terciaria:

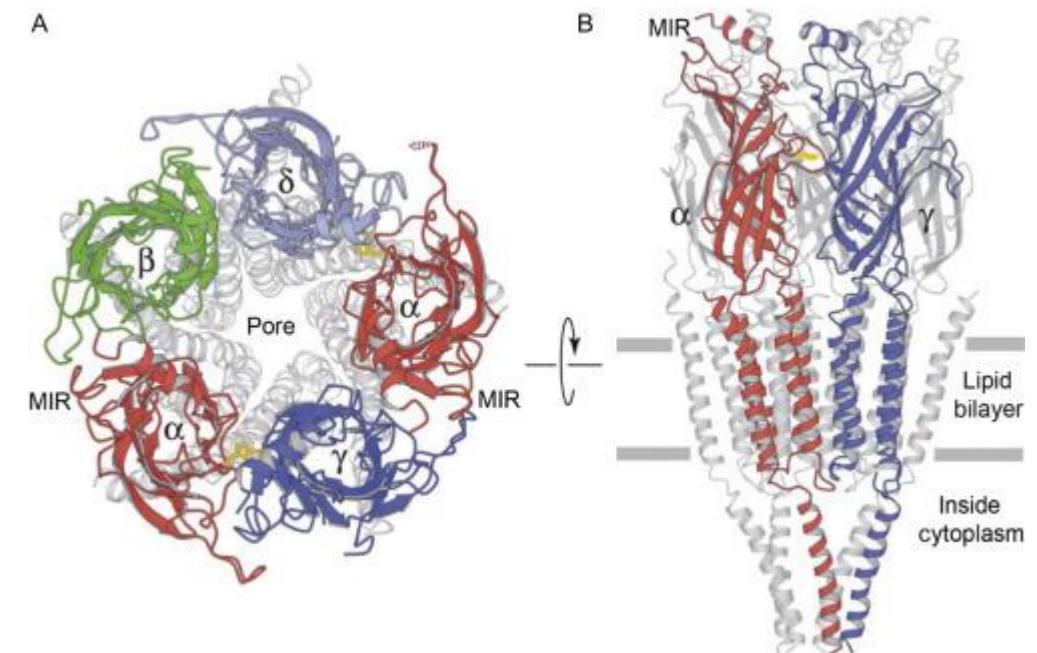
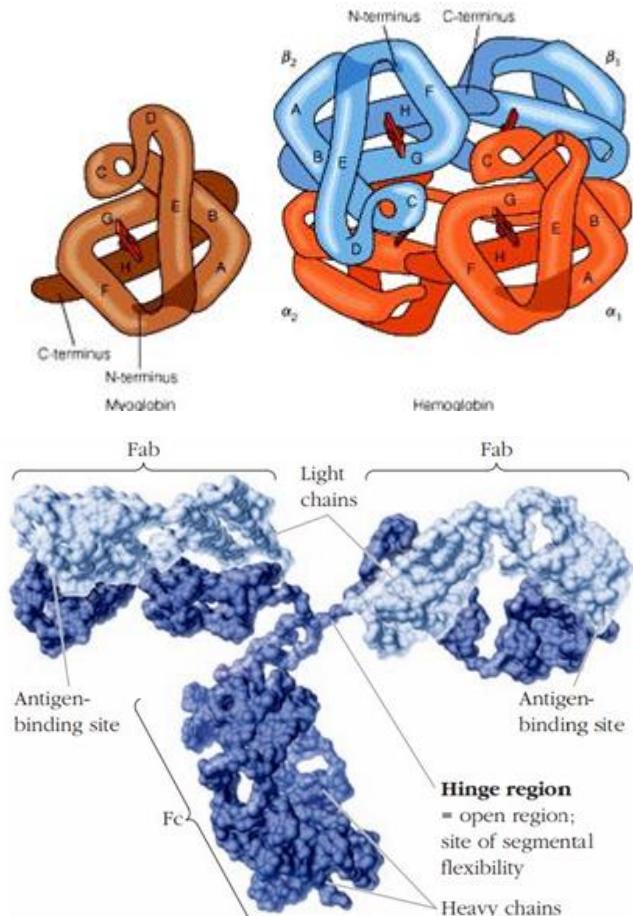
- **Dominios:** partes de la cadena polipeptídica estables de manera **independiente**, determinante de aspectos funcionales. Secuencia – estructura – función
 - **Efecto hidrofóbico** determinante en el plegamiento.
 - **Fuerzas de Van der Waals** en el núcleo.
 - **Puentes de hidrógeno** entre cadenas.
 - **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:

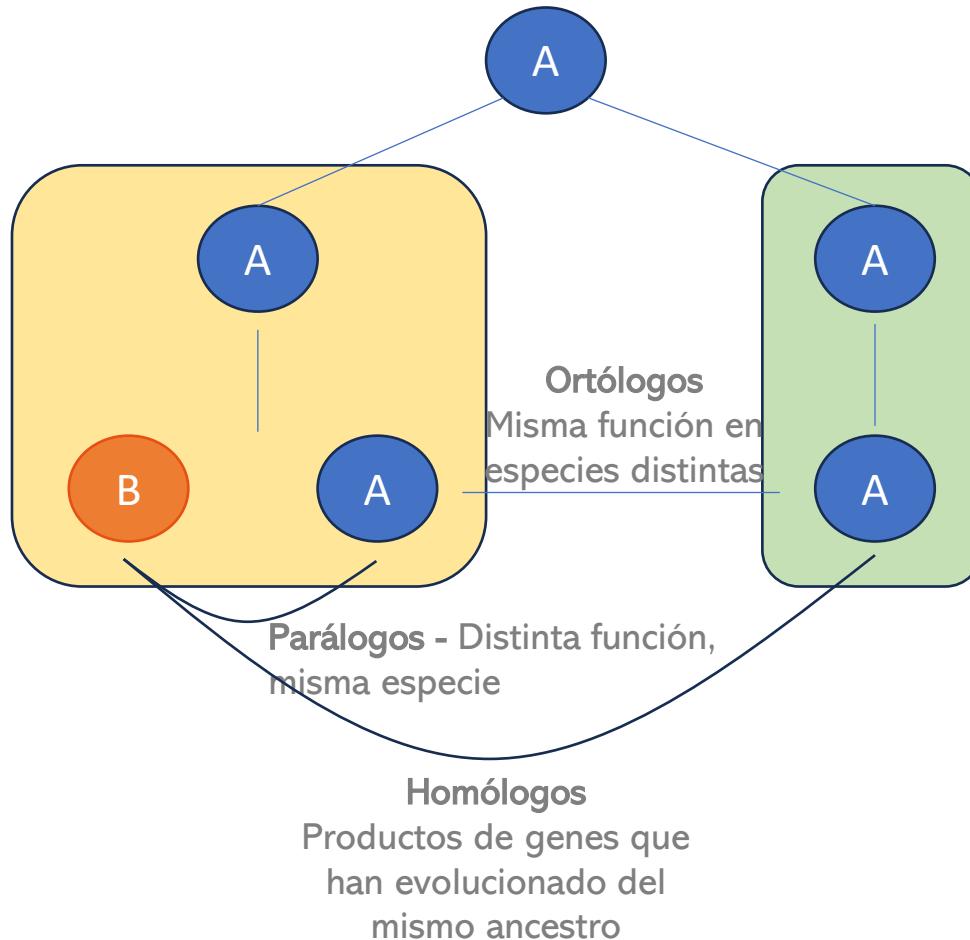
- Estructura cuaternaria: disposición de **varias** cadenas polipeptídicas
 - Dominio único vs multidominio (homo/hetero), proteínas de membrana



3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

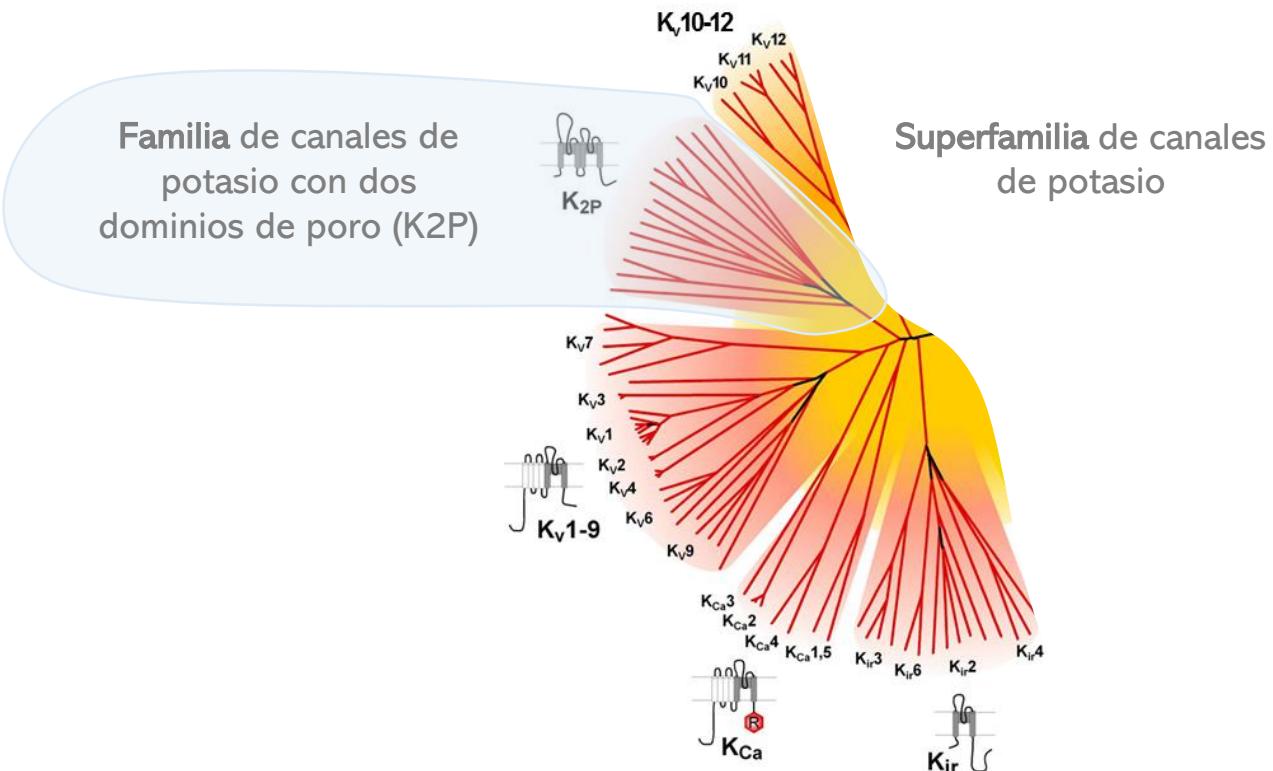
- Homología de proteínas: Homólogos - Ortólogos/Parálogos



3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

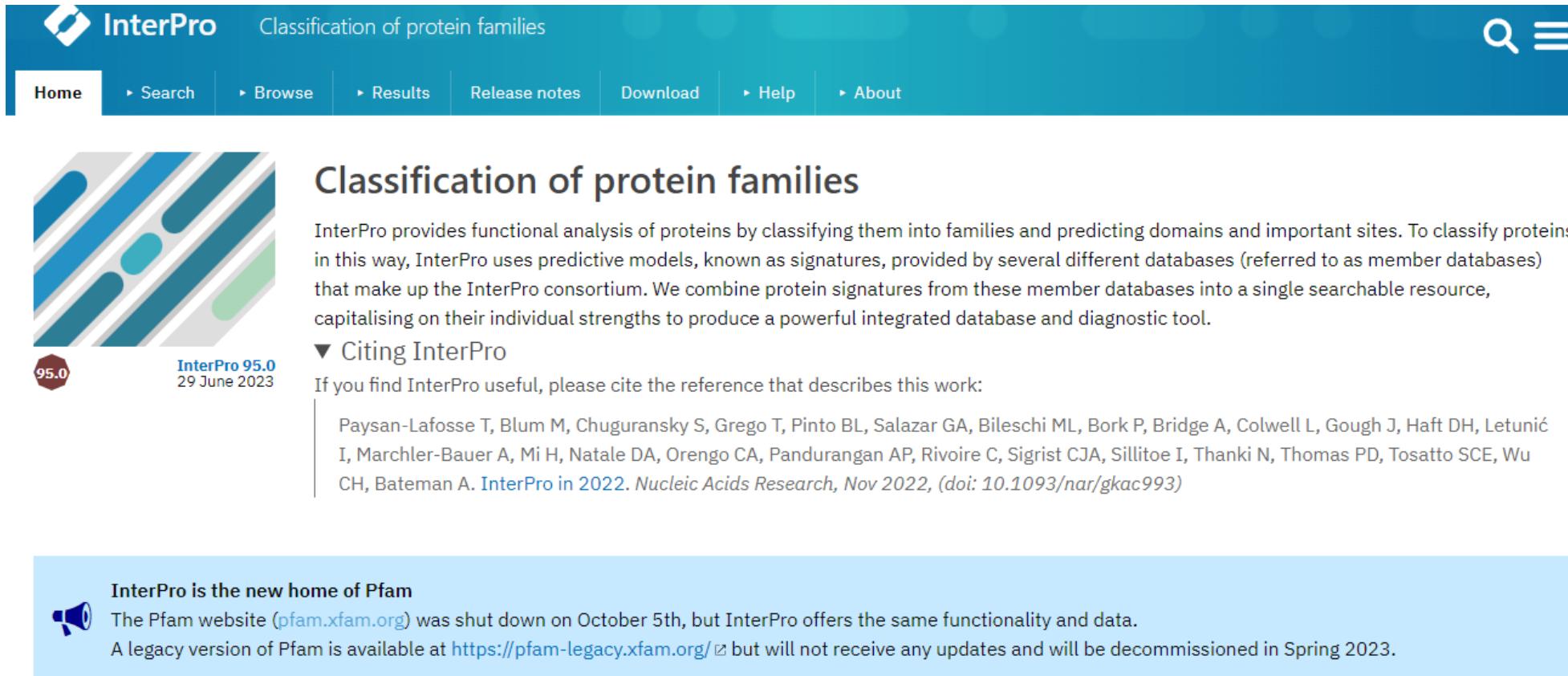
- **Familias proteicas:** son proteínas relacionadas por homología con una identidad de secuencia >30%, estructura y función similares
- **Superfamilias proteicas:** proteínas o dominios que tienen baja identidad de secuencia, pero presentan aspectos estructurales y funcionales similares.



3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

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

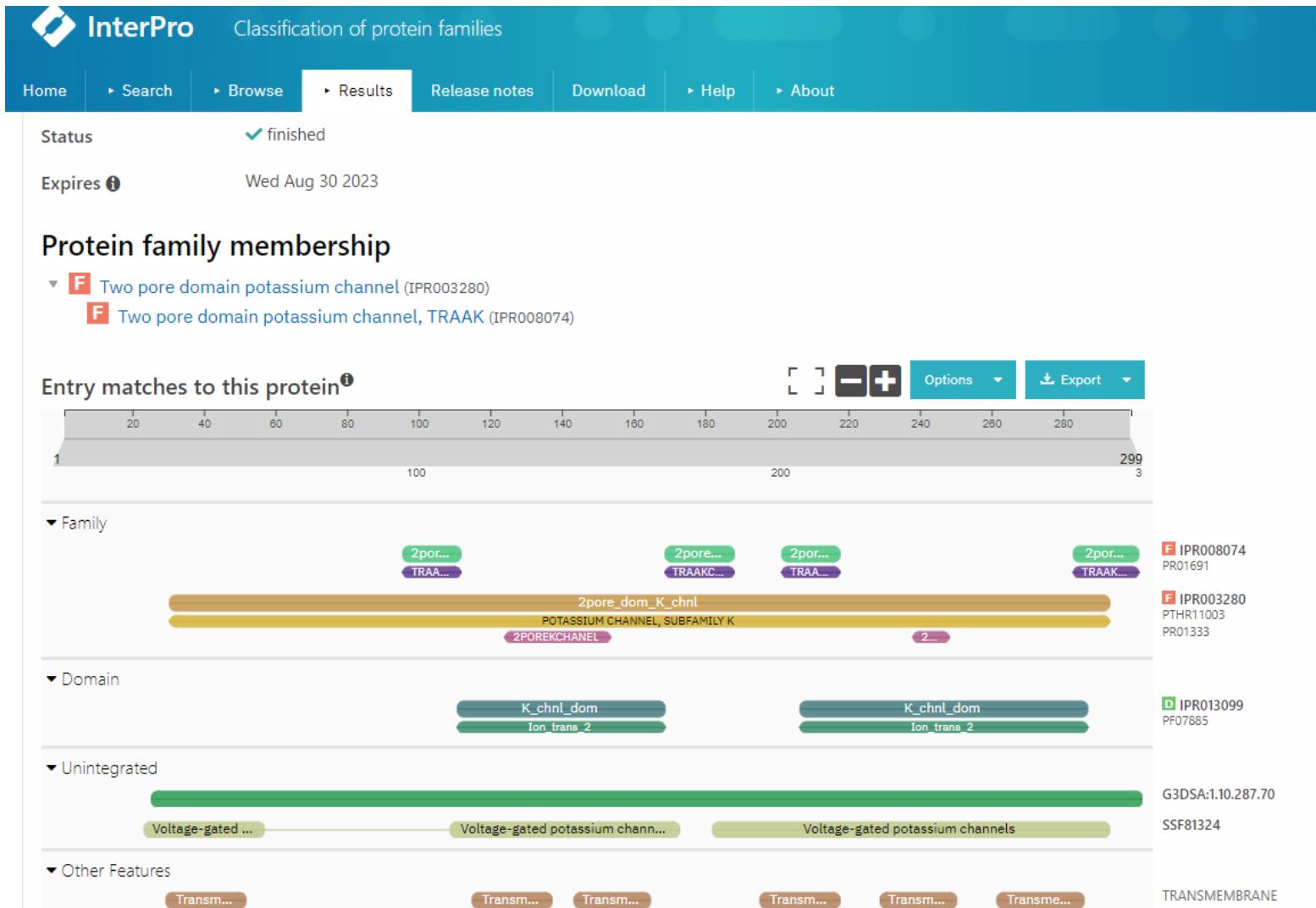


The screenshot shows the InterPro website homepage. The header features the InterPro logo and the text "Classification of protein families". The navigation bar includes links for Home, Search, Browse, Results, Release notes, Download, Help, and About. To the right of the navigation bar are search and filter icons. Below the header is a decorative graphic of overlapping blue and green shapes. On the left, there's a circular badge with "95.0" and the date "29 June 2023". The main content area is titled "Classification of protein families" and contains text explaining the tool's purpose: "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." A section titled "▼ Citing InterPro" provides citation information: "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, Bileshi ML, Bork P, Bridge A, Colwell L, Gough J, Haft DH, Letunic 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)". At the bottom, a blue banner states: "InterPro is the new home of Pfam. The Pfam website (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



3.1. Aspectos estructurales de las proteínas

Estructura de las proteínas:

- Recursos informáticos: PROSITE (prosite.expasy.org)

Database of protein domains, families and functional sites



SARS-CoV-2 relevant PROSITE motifs

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:



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]

ruler: 1 100 200 300 400 500 600 700 800 900 1000

USERSEQ1 (299 aa)

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:	GI11AG		
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](#)[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

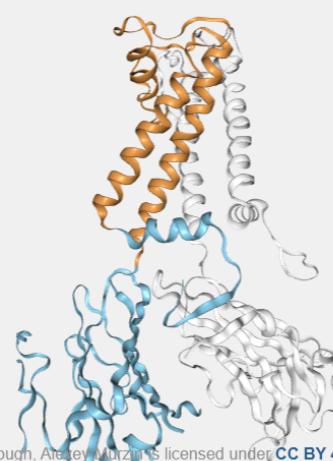
```
graph TD; A["class 1000000  
All alpha proteins"] --> B["fold 2000019  
Voltage-gated potassium channels"]; B --> C["superfamily 3000023  
Voltage-gated potassium channels"]; C --> D["family 4000034  
Voltage-gated potassium channels"]; D --> E["domain 8003429"]
```

Representative sequence Other domains for this sequence External links

UniProt P83698
This domain

MNIVDPFSPHS SDSFAQAQASP ARKPPRGRR IWSGTREVIA YGMPASVWRD LYIWALKVSW PVFFASLAA L YQLQGDAPIA NQSPPGFVG A FFFSVETLAT VGYGDMHPQT VYAHAIATLE IFVGMSGIAL STGLVPARFA RPRAKIMFAR HAIVRPFNGR MTLMVRAANA RQNVIAEARA KMRILMRREHS SEGYSLMKIH DLKLVRNEHP IFLLGWNMMH VIDESSPLFG ETPESLAEGR AMLLVMEGS DETTAQVMQA RHAWEHDDIR WHHRYVDLMS DVDGTHIDY TRFDNDTEPV E PPGAAPDAQA FAAKPGEFDA RPV

Legend:
■ 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, Atley Muzzenich licensed under CC BY 4.0

Build 1.0.6

Temario - Contenidos

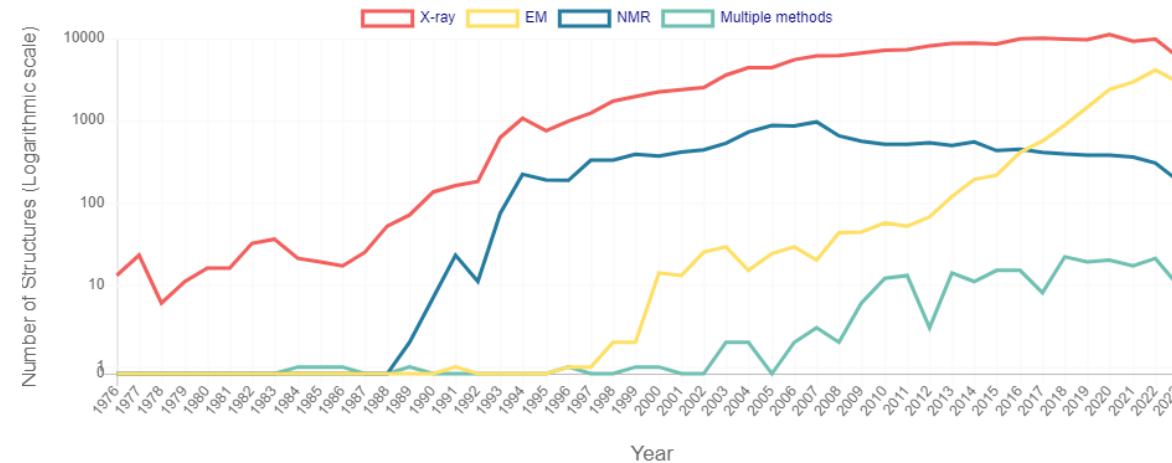
Tema 3. Proteómica estructural

- 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 crioelectrónica 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.BORGNA,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.BORGNA,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
REMARK 350
```

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	CA	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

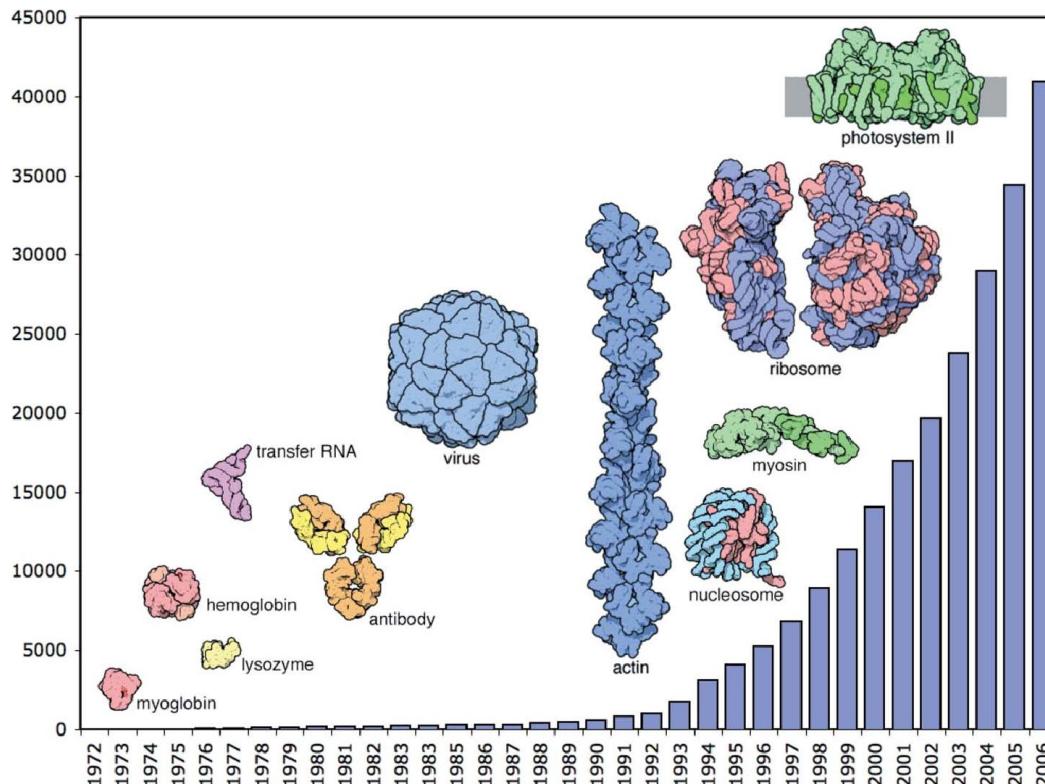


Figure 1

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
Takeda, Janssen, Boehringer Ingelheim, Pfizer, MERCK, Bristol Myers Squibb, A Member of the Roche Group

6 Research Sites
UNIVERSITY OF TORONTO, THE UNIVERSITY of NORTH CAROLINA at CHAPEL HILL, Karolinska Institutet, GOETHE UNIVERSITÄT FRANKFURT AM MAIN, McGill UNIVERSITY, UCL

Major Funding Supporters Include
Wellcome, IMI, Innovative Medicines Initiative, NIH, BILL & MELINDA GATES foundation, Mitacs, CIHR IRSC, GenomeCanada

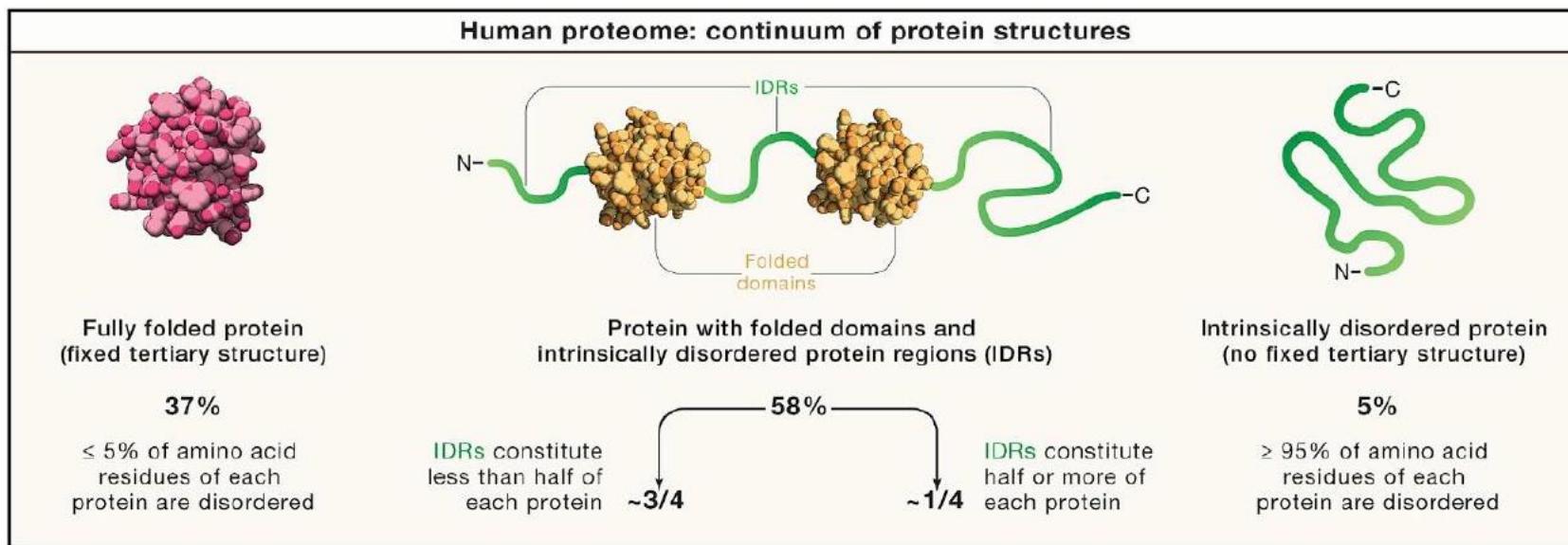
330+ Partnerships
25+ Publications with industry partners each year

3.2. Métodos de caracterización estructural

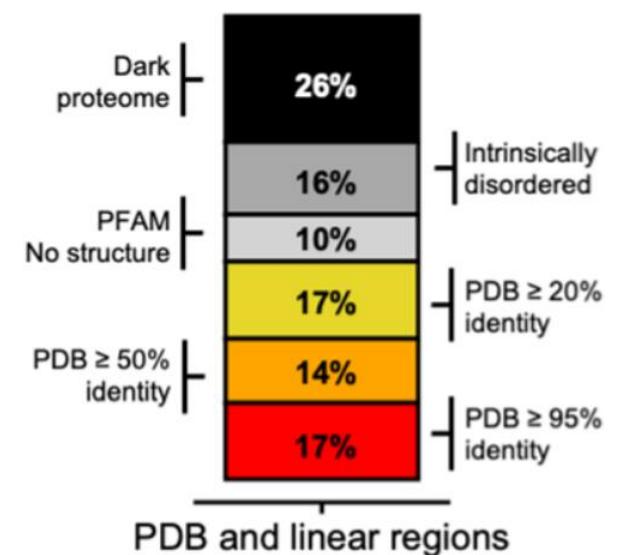
El proteoma estructural humano:

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)

CATH / Gene3D v4.3

151 million protein domains classified into 5,841 superfamilies

Search by keywords, PDB code, GO term, etc

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

Protein Evolution
Learn about a particular protein family and how it evolved

Protein Function
Investigate the function of your protein

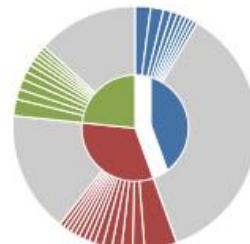
Conserved Sites
Look at protein sites that are highly conserved and implicated in function

Download Data
Download data files and query CATH via webservices

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

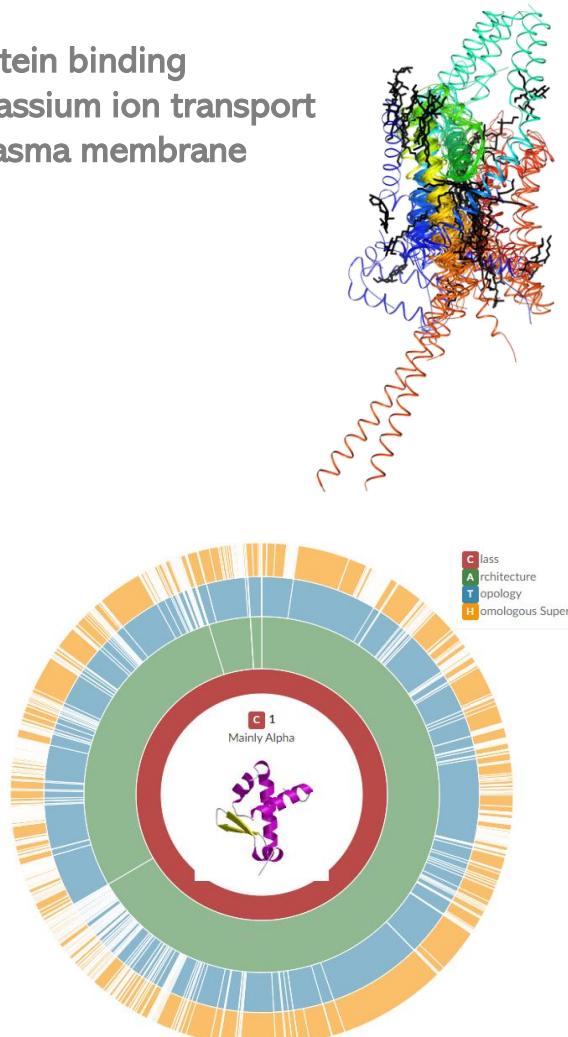
ID	Function Family (FunFam) Name	Total Sequences	Enzyme?	Structure?	Structural Representative	PDB Sites?	Diversity (0-100)
1	Sodium channel protein	2092	-	-	-	84.7	
2	Potassium voltage-gated channel subfamily a member	1878	3D	4jtdH03	-	96.2	

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



CATH Classification

Level	CATH Code	Description
C	1	Mainly Alpha
A	1.10	Orthogonal Bundle
T	1.10.287	Helix Hairpins
H	1.10.287.70	

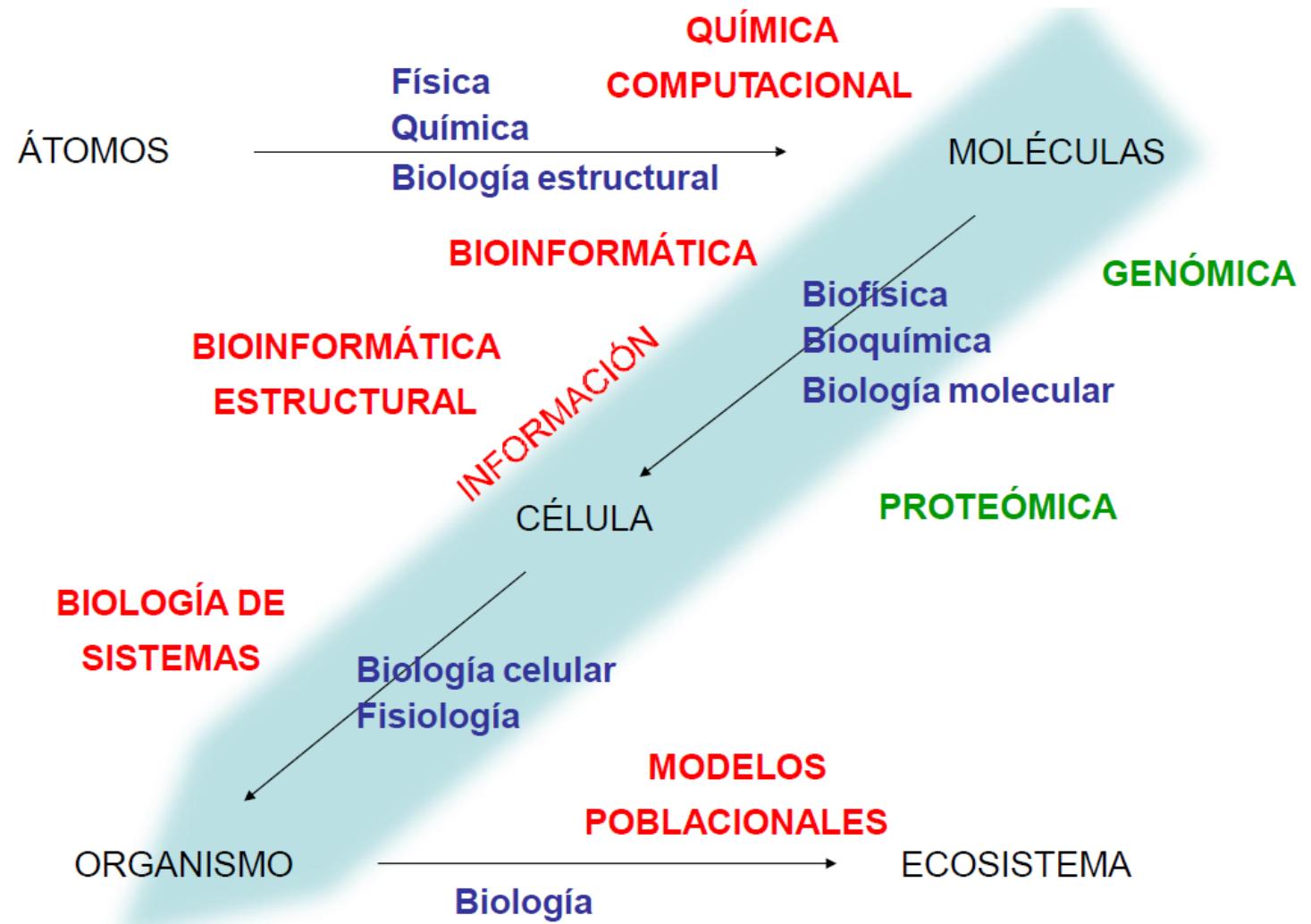


Temario - Contenidos

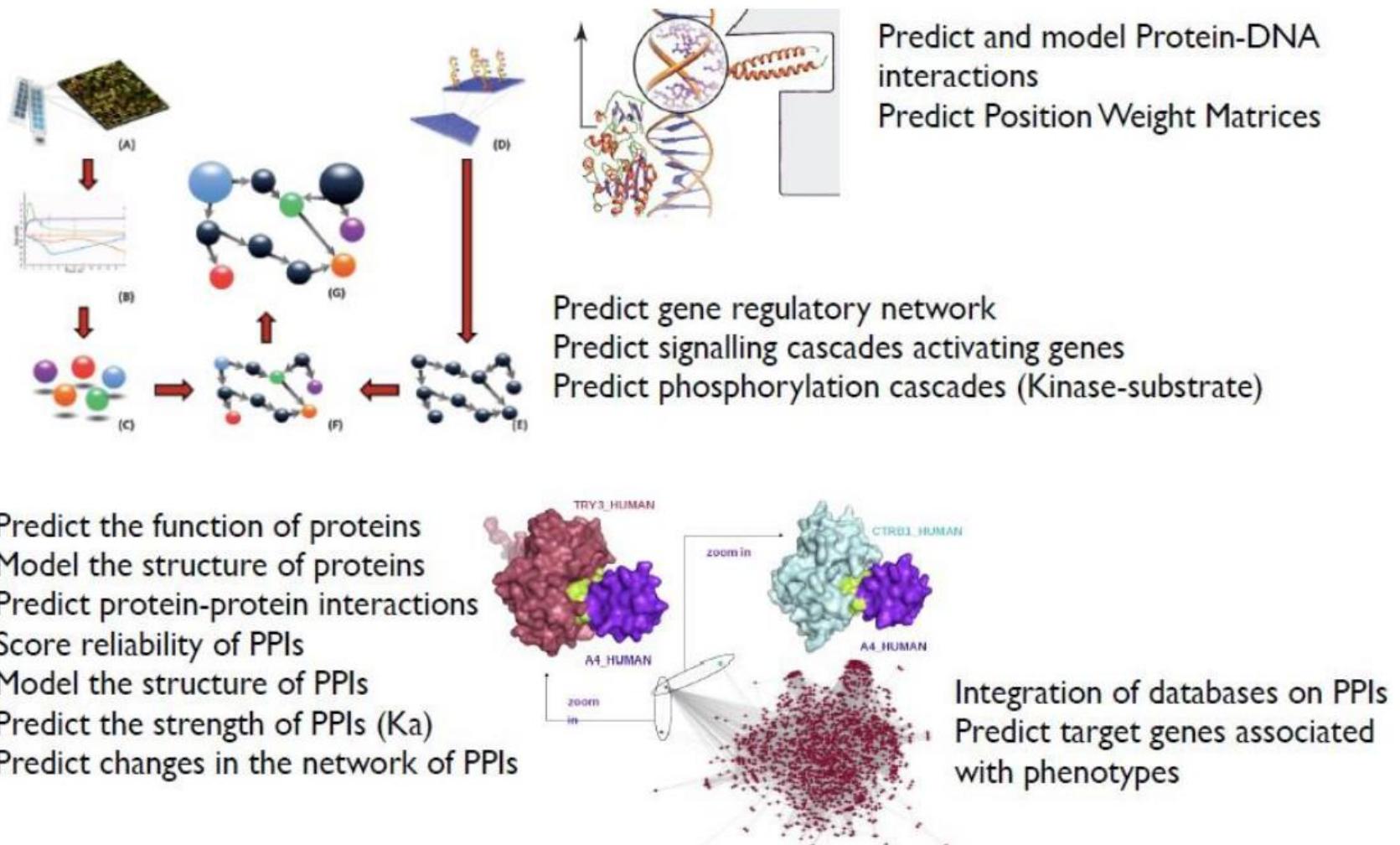
Tema 3. Proteómica estructural

- 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**

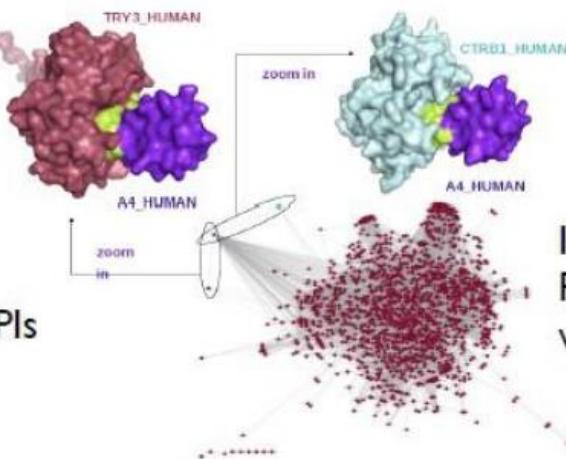
3.4. Bioinformática estructural



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

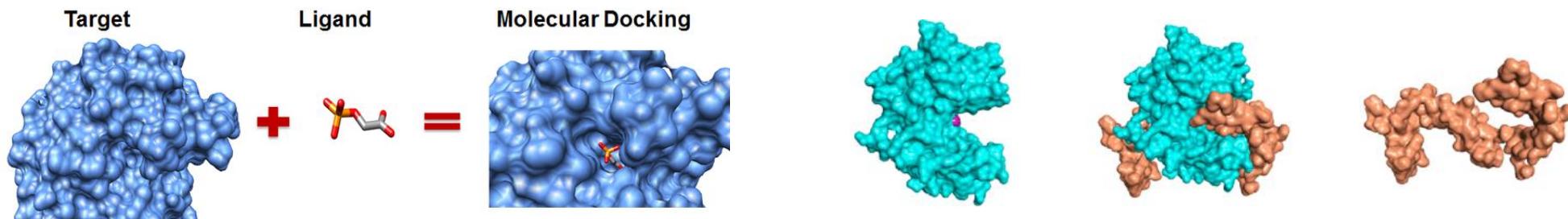


Integration of databases on PPIs
Predict target genes associated with phenotypes

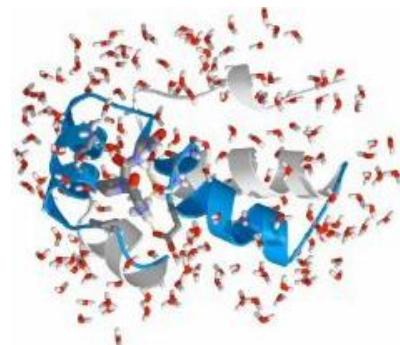
3.4. Bioinformática estructural

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





viu

**Universidad
Internacional
de Valencia**

universidadviu.com

De:
 Planeta Formación y Universidades