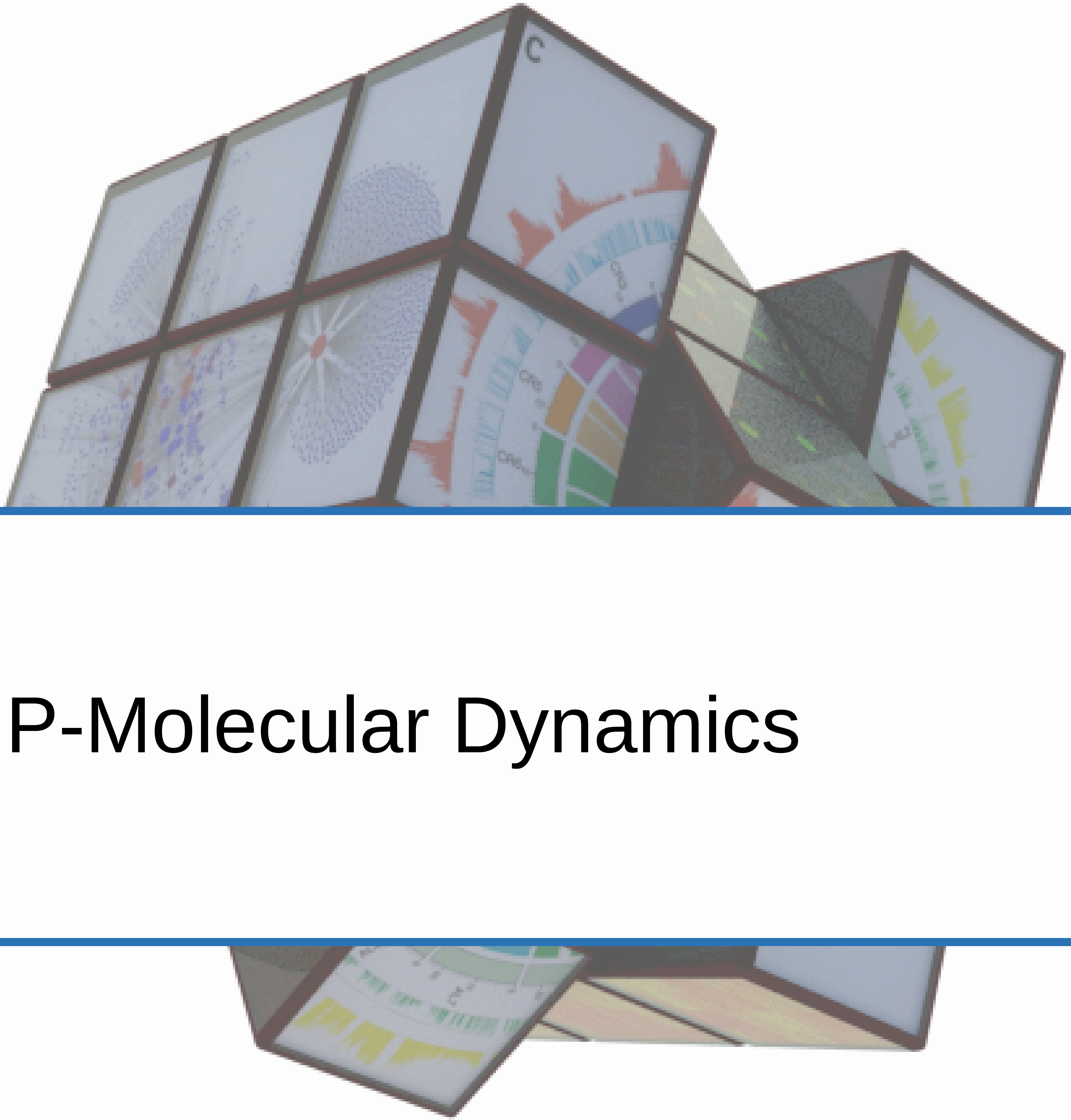


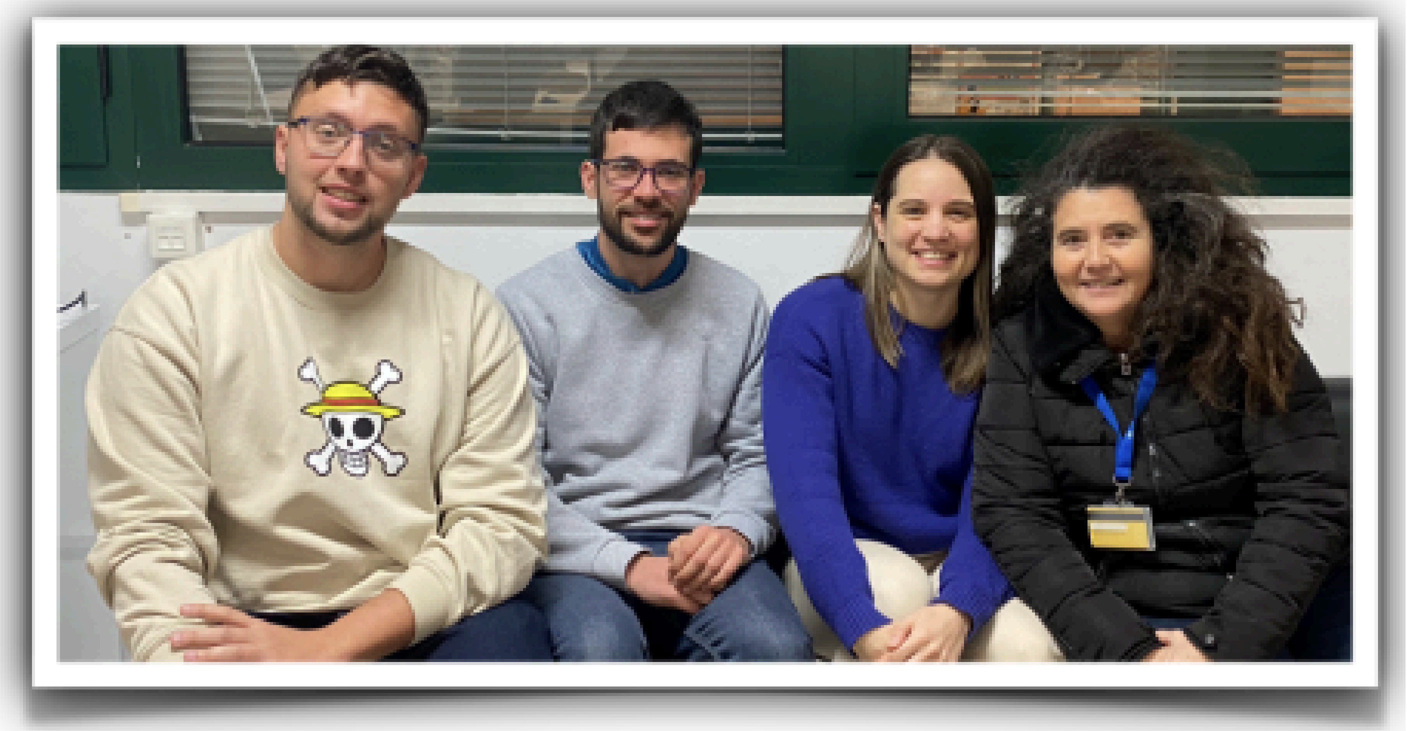
P-Molecular Dynamics

Francisco Miguel Pérez Canales 21th BMWC

CBBio

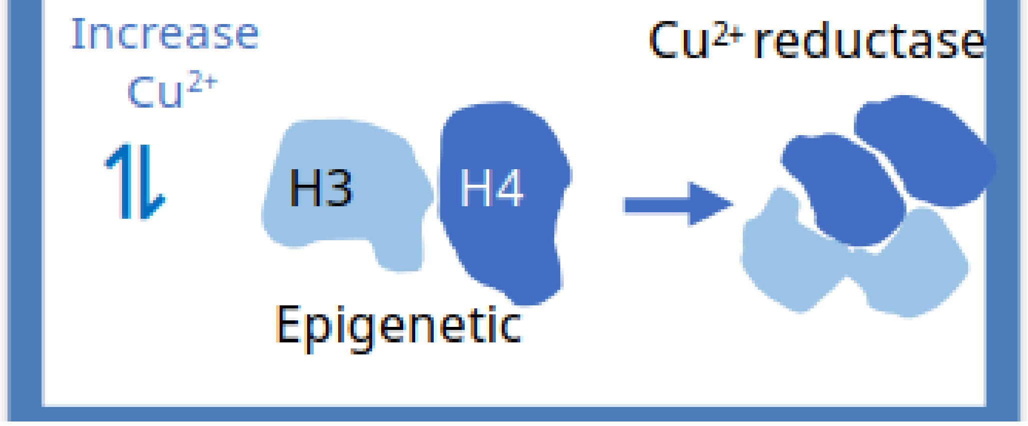
Projects and Colaborators

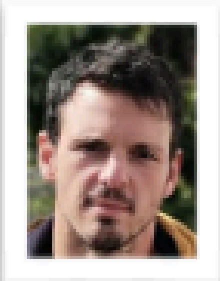
FUNCTION



Metamorphism

Moonlighting

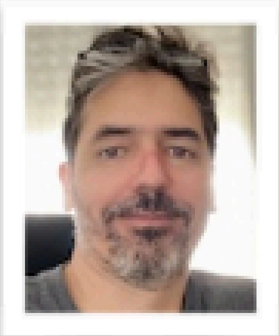




MINISTERIO
DE CIENCIA
E INNOVACIÓN

AGENCIA
ESTATAL DE
INVESTIGACIÓN

Ildefonso Cases
(Bioinfo. Unit)
MdM platform



ANNOTATION

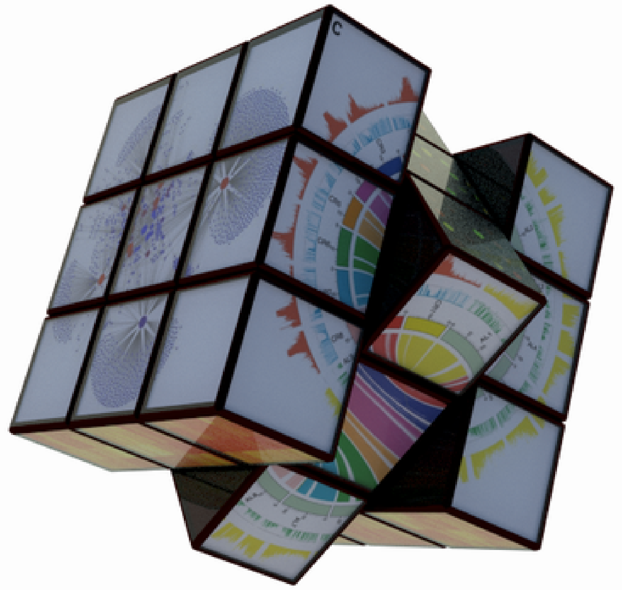
ERGA

A GENOME ATLAS
OF EUROPEAN
BIODIVERSITY

Projects and Colaborators

UNIVERSIDAD DE SEVILLA

Escuela Técnica Superior de
Ingeniería Informática



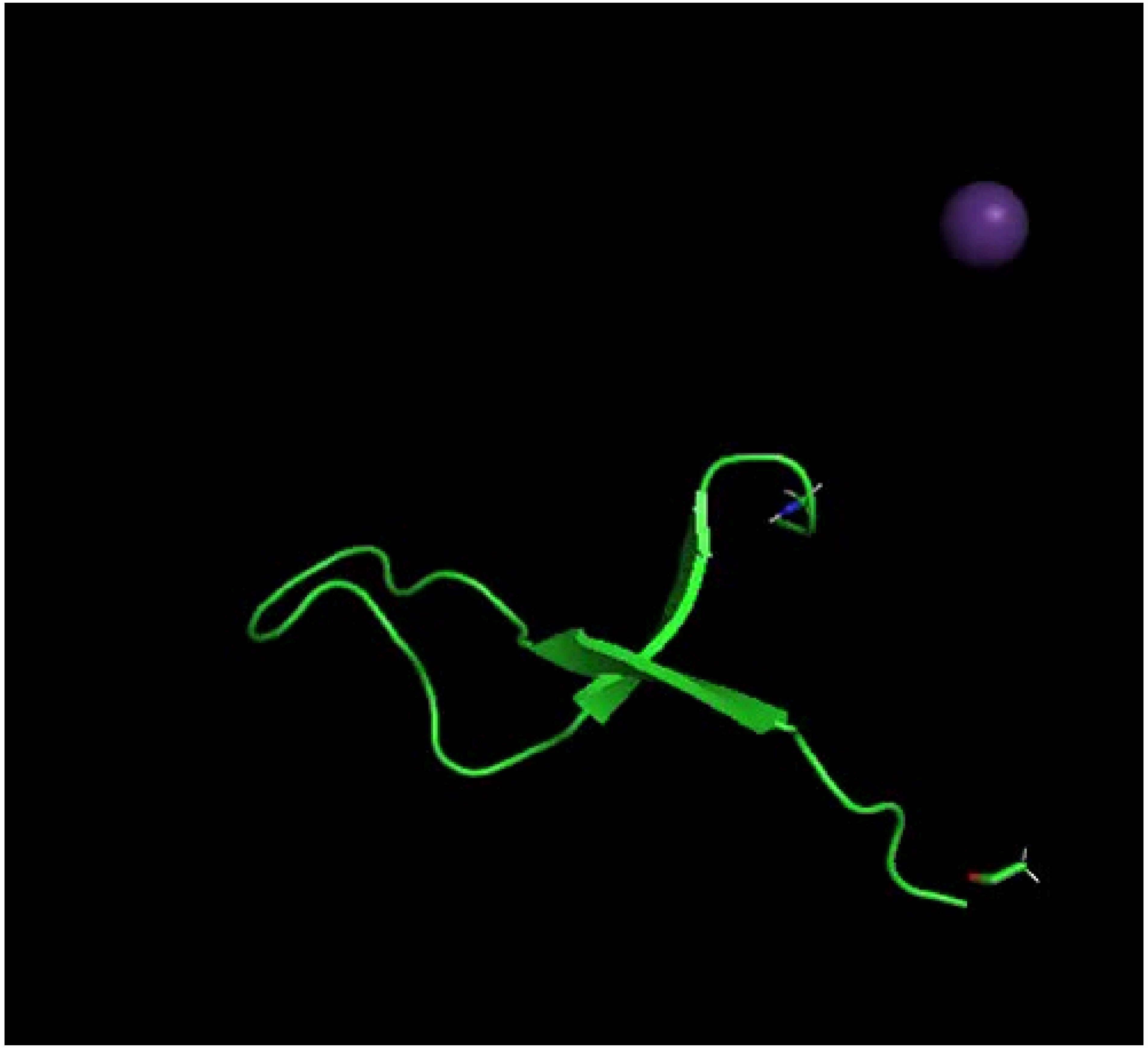
CSIC
CONSEJO SUPERIOR DE INVESTIGACIONES CIENTÍFICAS

RGNC

Molecular Dynamics

A computational technique that simulates the movement of atoms and molecules over time.

Molecular Dynamics Sample

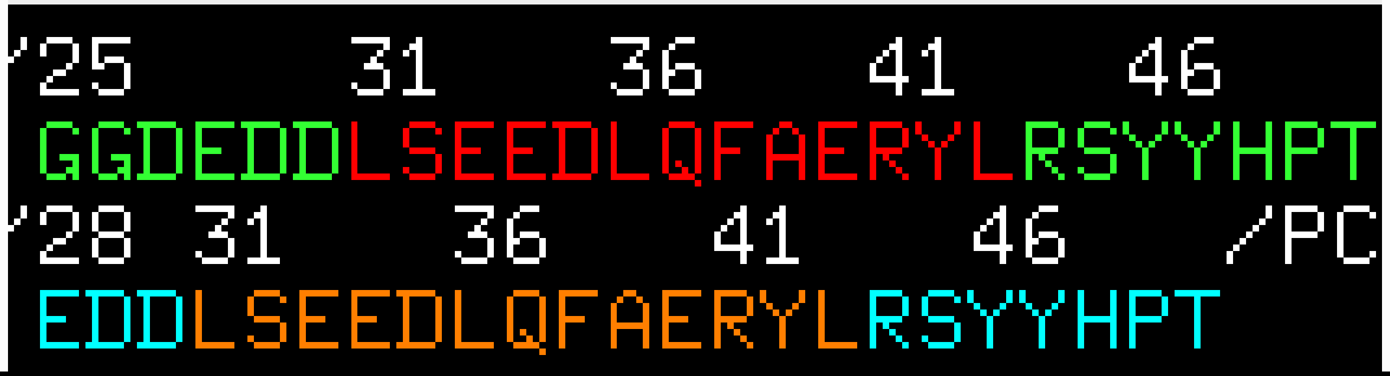


Proteomics

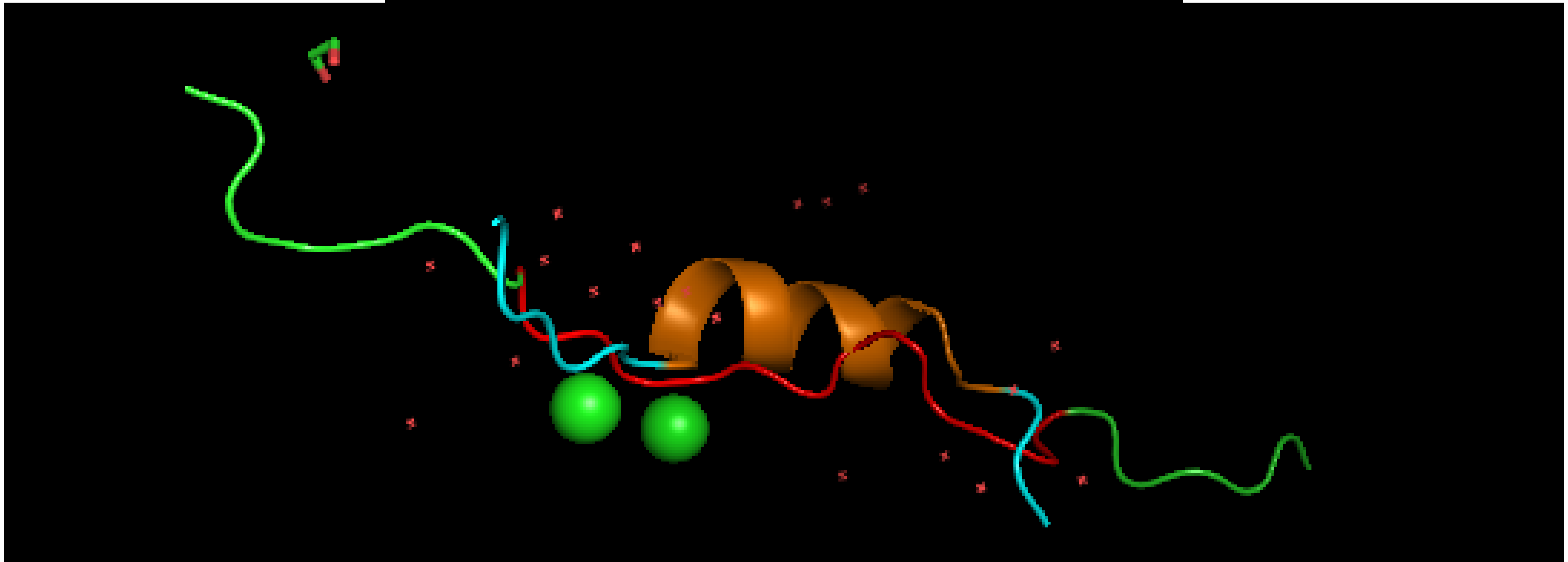
Molecular Dynamics Complexity

- **Configuration space**: Exponentially large atomic arrangements are hard to explore.
- **Energy minimization**: Finding global minima is NP-hard.
- **Trajectories**: Simulations cover only small configuration subsets.

What I do research



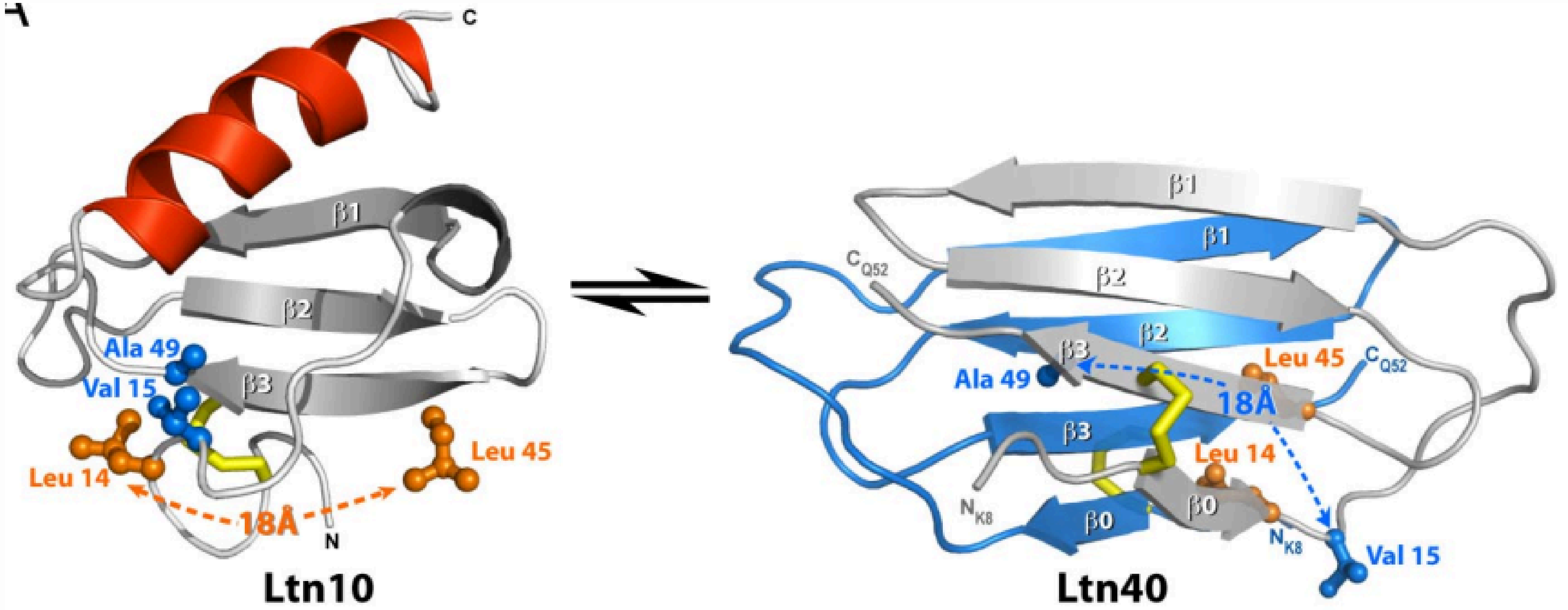
```
25      31    36    41    46
GGDEDDLSEEDLQFAERYLRSYYHPT
28 31    36    41    46    /PC
EDDLSEEDLQFAERYLRSYYHPT
```



Secondary Structure

Proposed Problem

Given two stable structural conformations, what are the potential intermediate states enabling the transition between them?

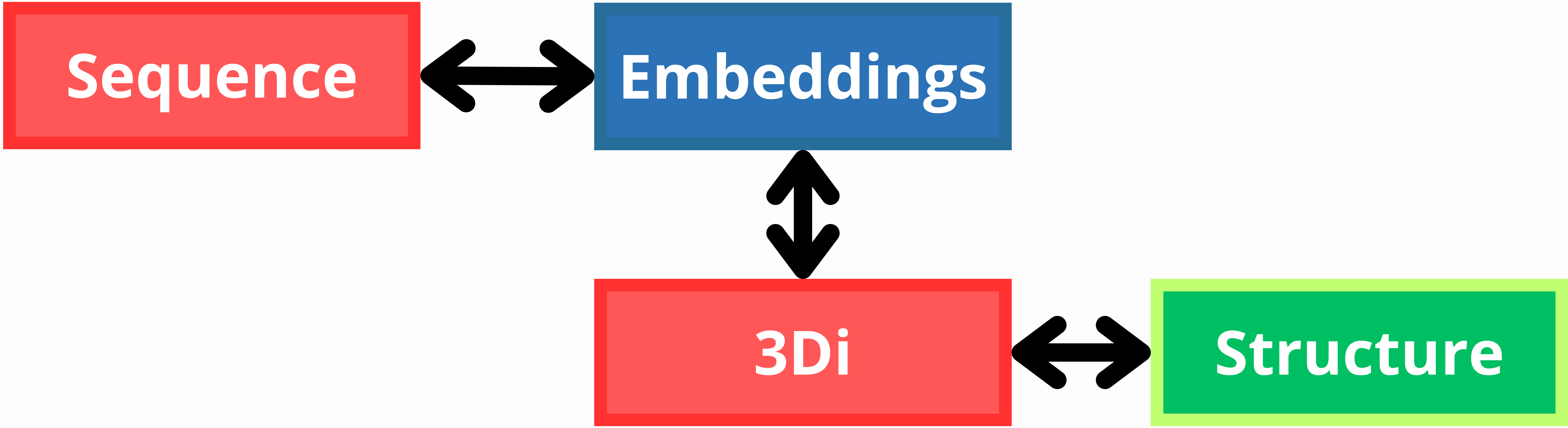


Interconversion between two unrelated protein folds in the lymphotactin native state | PNAS

Simplifying the problem

Protein Language Models?

Encoding and decoding between different formats



Sequence

Embeddings

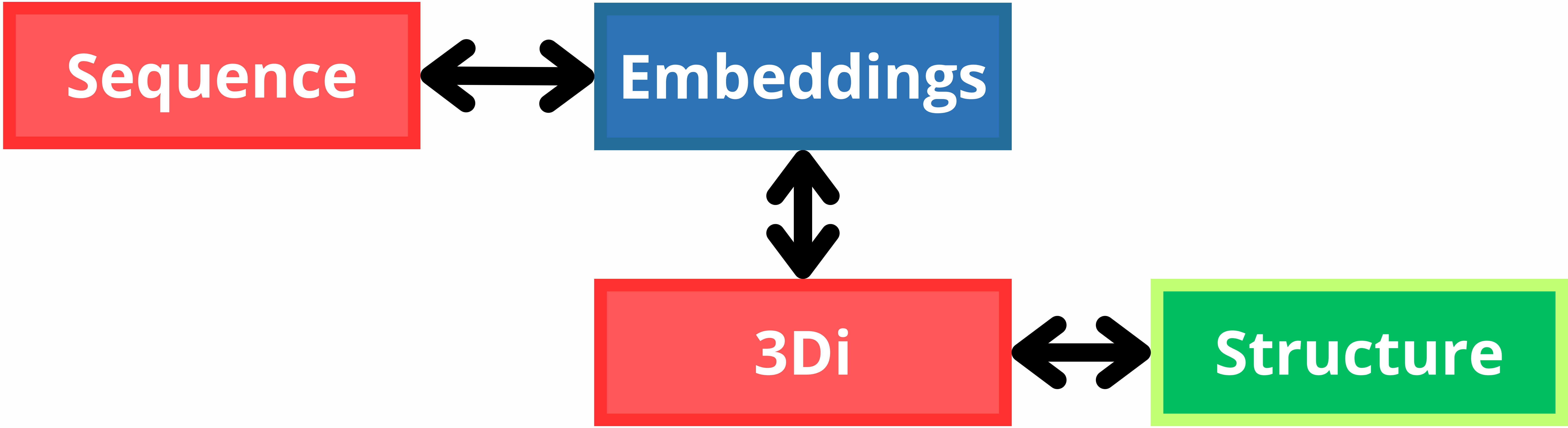
3Di

Structure

References: FOLDSEEK - ProstT5

Protein Language Models?

Encoding and decoding between different formats



Sequence

Embeddings

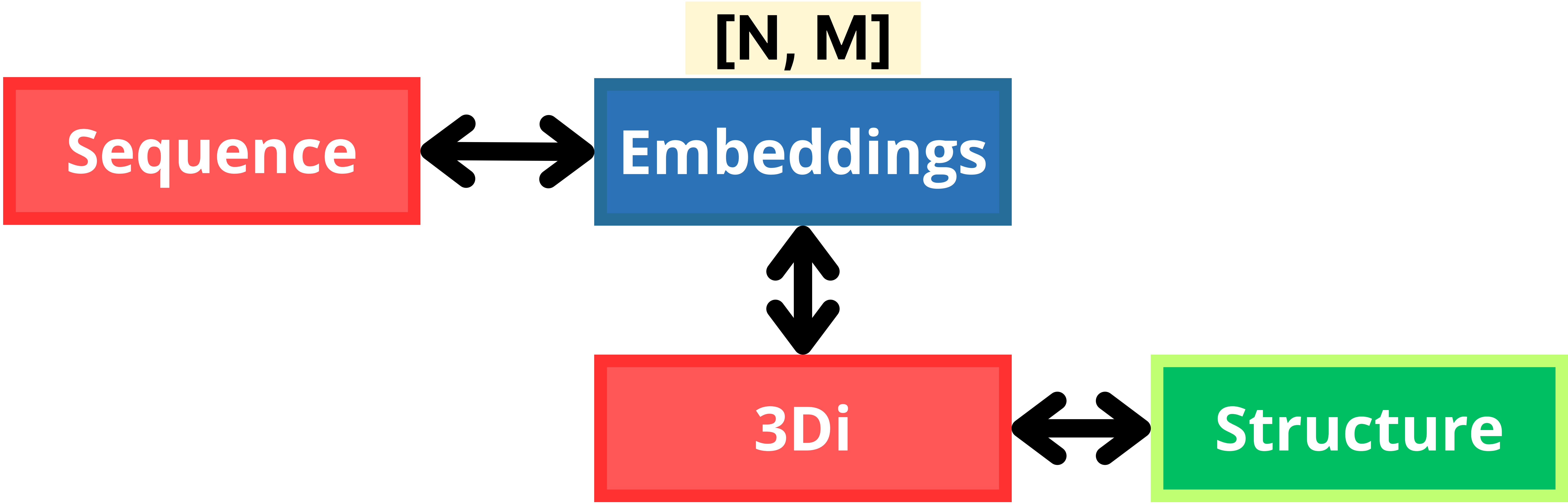
3Di

Structure

lead to shifts in significance

Protein Language Models

We have numbers for calculous



[N, M]

Sequence

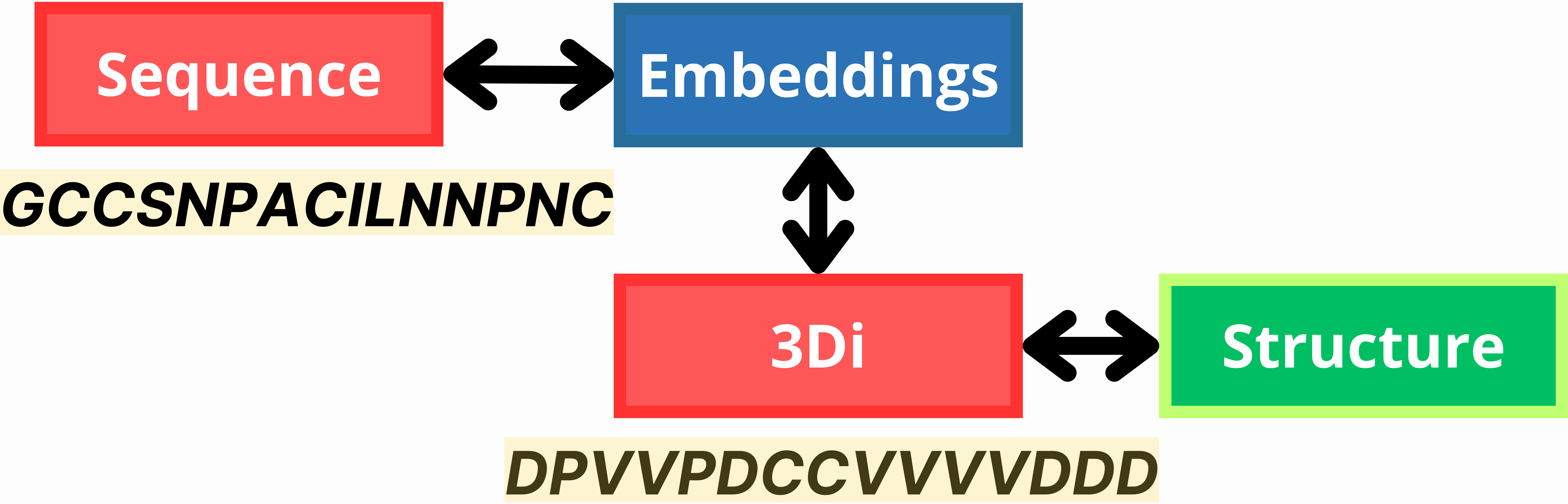
Embeddings

3Di

Structure

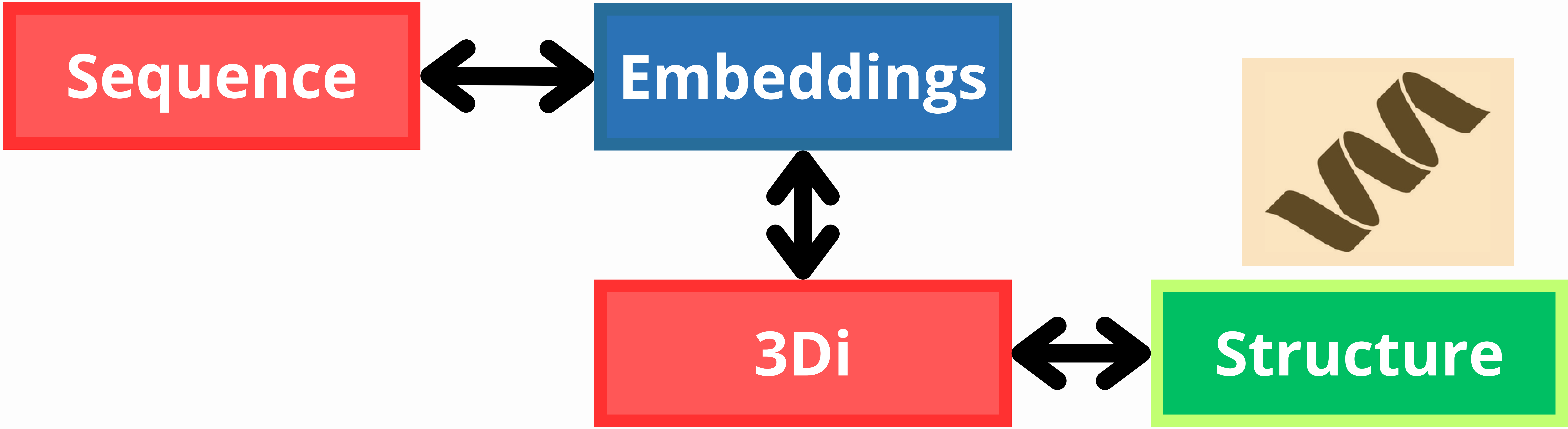
Protein Language Models

we have sequences



Protein Language Models

Structure are 3D atoms collection



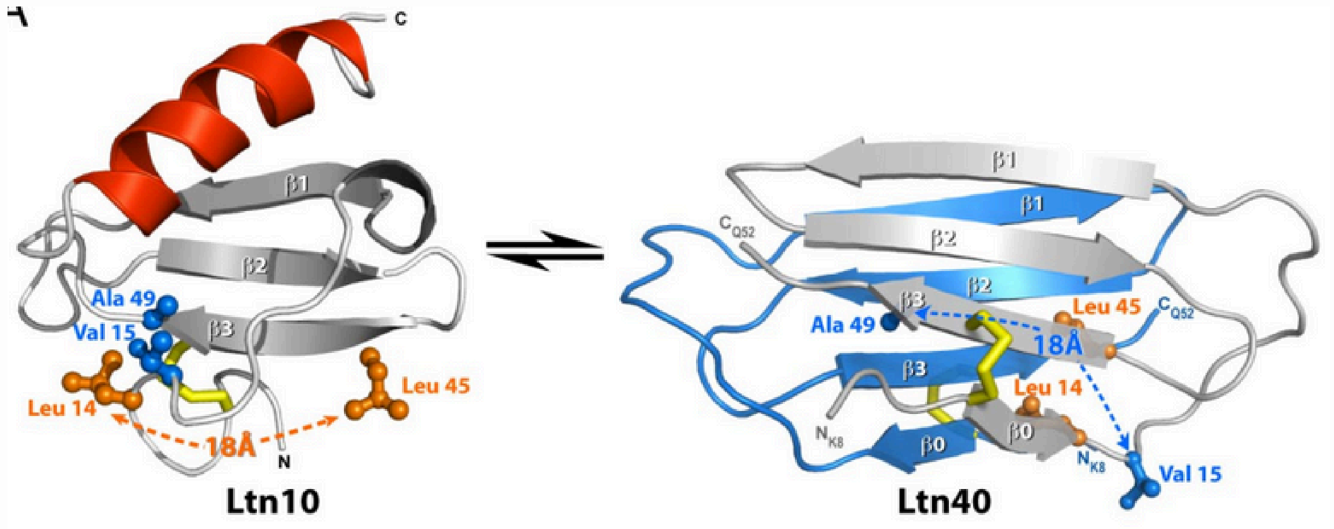
Sequence

Embeddings

3Di

Structure

Simplified Problem



DPVVPDCCVVVVDDD

VDVVPDCCPPVVDDD

Brief Definition Attempt

$$
\begin{aligned}
A &= \{A, R, N, D, C, Q, E, G, H, I, L, K, M, F, P, S, T, W, Y, V\},\\
S &= (s_1, \ldots, s_n) \quad (s_i \in A),\\
\Omega &= (\text{feasible structural space for } S),\\
M &= (m_1, m_2) \quad (m_1, m_2 \in \Omega),\\
3Di\_struct &= T(M), \quad M' = \widehat{T}(3Di\_struct),\\
\text{Goal: Find } M' &= (m_1^0, \ldots, m_1^k) \text{ s.t. } m_1^0 = m_1,\ m_1^k = m_2,\ m_1^i \in \Omega\, \forall\, 0 \le i \le k.
\end{aligned}
$$

Thanks

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