DSIMB
DYNAMICS OF STRUCTURES AND INTERACTIONS OF BIOLOGICAL MACROMOLECULES

La recherche au DSIMB

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Laboratoire DSIMB

Dynamique des Structures et Interactions
des Macromolécules Biologiques
UMR-S 1134 Biologie Intégrée du Globule Rouge
INSERM, Univ. Paris Cité, Univ. Réunion

Inserm
La science pour la santé
From science to health

UR | UNIVERSITÉ DE LA RÉUNION

Université Paris Cité

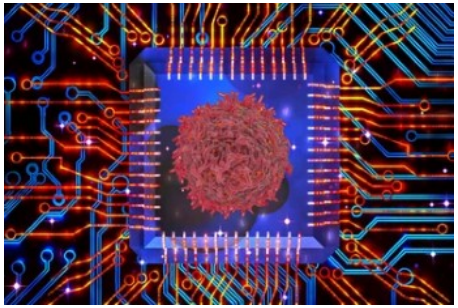
DSIMB

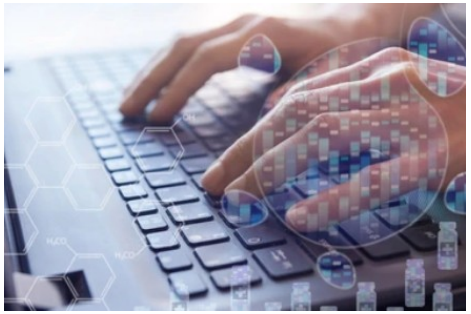
Equipe Bioinformatique de l'unité Inserm u1134

Prédictions Structurales

Simulations Moléculaires

Développements Méthodologiques





DSIMB

Effectif : 11 chercheurs/enseignants-chercheurs (permanents)

6 doctorants

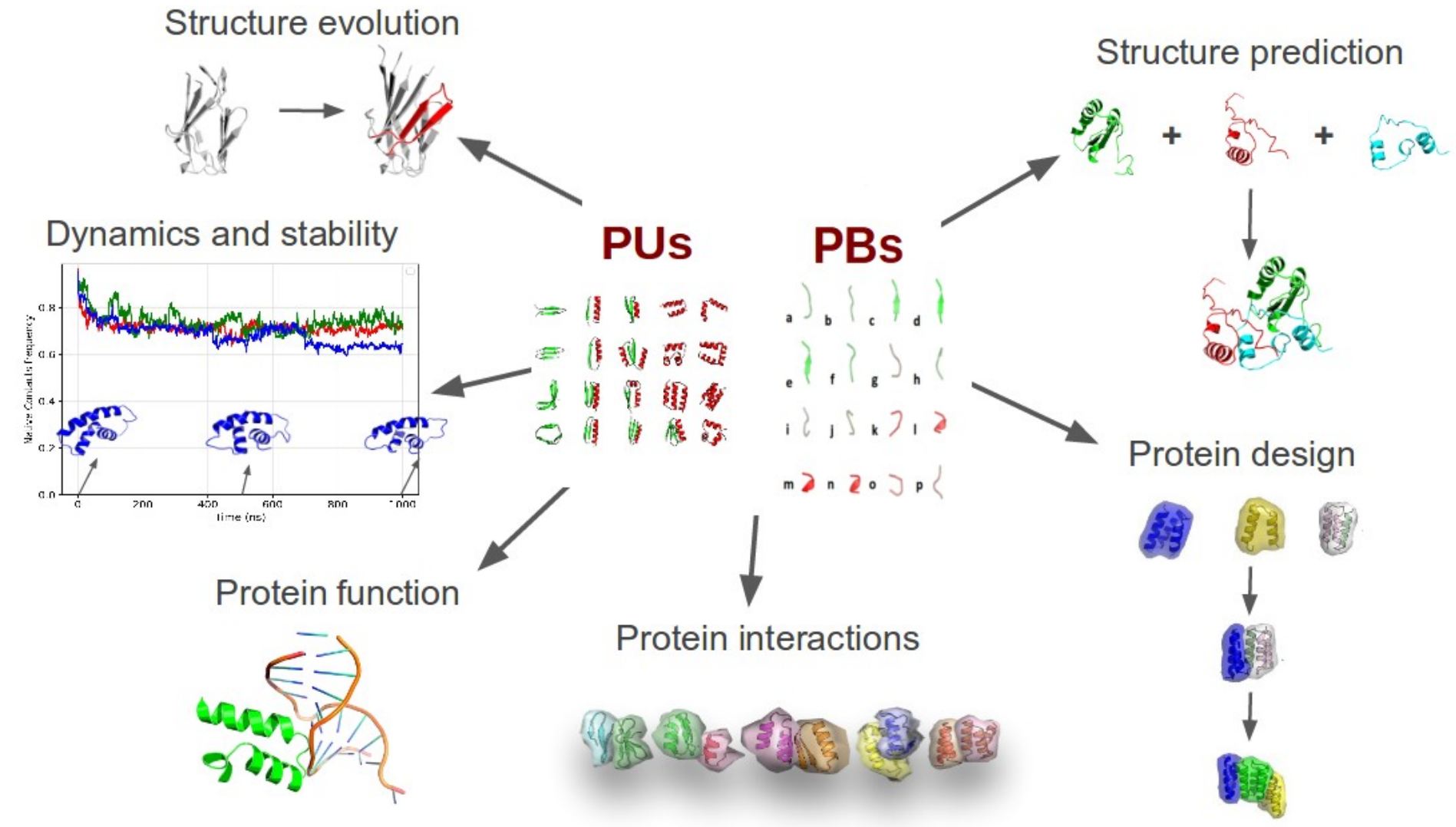
Collaborations quasi-systématiques avec expérimentateurs

Expertises : Bioinformatique, Biochimie, Chimie, Mathématiques

Thèmes principaux :

- Comprendre la relation séquence-structure-fonction
- Modéliser et simuler des protéines dans leur environnement
- Développer des molécules à visée thérapeutique
- Prédire grâce à l'apprentissage profond et à l'approche multimodale
- Modéliser des voies métaboliques

Comprendre la relation séquence-structure-fonction



Comprendre la relation séquence-structure-fonction

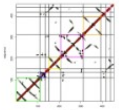
STRUCTURE ANALYSIS

SWORD2
SWift and Optimized Recognition of protein Domains

An automated method that identifies protein domains using information on protein internal contacts between the residues.

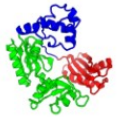
MEDUSA
Multiclass flexibility prediction from sequences of amino acids

MEDUSA is a Deep Learning approach for prediction of protein flexibility from sequence.



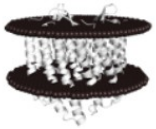
Protein Peeling 3
Peel a protein

An approach for splitting a 3D protein structure into compact fragments.



SWORD
SWift and Optimized Recognition of structural Domains

A partitioning algorithm capable of producing multiple alternative domain assignments for a given protein structure.

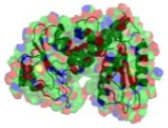


OREMPRO
ORientation and Evaluation of Membrane PROteins

A tool for the structural assessment of protein transmembrane domains.

Protein Block Expert
Web-based protein structure analysis server using a structural alphabet

PBE server 2.0 aims to provide a platform for protein structure analysis and comparison using well defined library of short structural motifs (SSMs) known as structural alphabets (SA).



VLDP
Determine protein contacts, accessibility and residue volume using Laguerre diagram

VLDPws is a tool for analysing protein structures based on Laguerre diagram, a powerful mathematical-geometric method.

SPECIALIZED DATABASES

RHeference
Database dedicated to RH alleles, focusing on RHD alleles and RHCE alleles expressing D epitopes

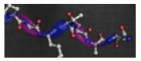
RHeference provides an overview of current knowledge regarding these alleles and an easy access to all relevant information for each allele.

CALR-ETdb
Calreticulin variant database involved in essential thrombocythemia

This project aims to compile all the variants of Calreticulin involved in essential thrombocythemia within the same database, namely CALR-ETdb.

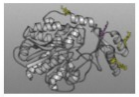
RESPIRE
Repository of Enhanced Structures of Proteins Involved in the Red blood cell Environment

This database aims at providing a reference, ordered and protein-driven information on proteins available in the erythrocyte.



PolyprOnline
A database dedicated to Polyproline II Helix conformations in proteins

PolyprOnline is a requestable database dedicated to the assignment of PolyProline II helices.



PTM-SD
Post Translational Modification Structural Database

PTM-SD provides an access to proteins for which Post Translational Modifications are both experimentally annotated and structurally resolved.

MitoGenesisDB
Mitochondrial Spatio-Temporal Expression Database

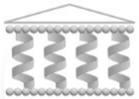
The database MitoGenesisDB focuses on the dynamic of mitochondrial protein formation through global mRNA analyses.

PB-PENTAdb
Database of pentapeptides from protein structures

A platform to investigate the structural features of pentapeptides in protein structures.

KNOTTIN
KNOTTIN database

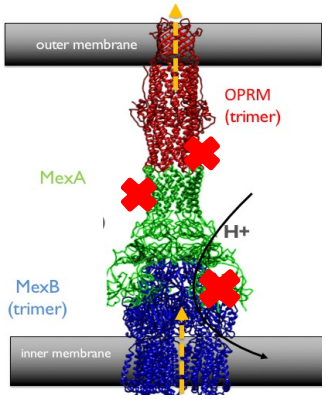
Knottins are small disulfide-rich proteins characterized by a very special "disulfide through disulfide knot"



TMPL
TMPL database

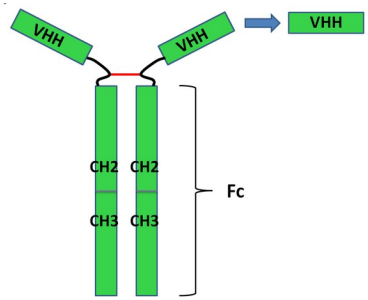
Transmembrane protein Models Positioned in the Lipid bilayer

Modéliser et Simuler des Protéines



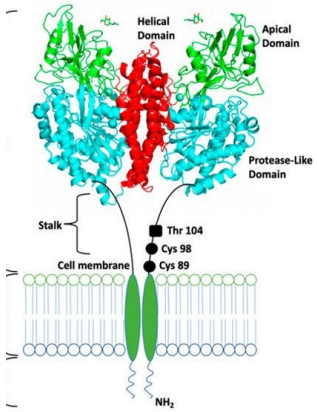
► Inhibiteur de l'assemblage des protéines responsables de l'efflux des antibiotiques

- Anne-Elisabeth Molza (ingénieur)
- Fatiha-Ikram Lalaimia (ingénieur)
- Clément Moroldo (ingénieur)



► Structures et dynamiques des nanobodies VHH

- Aravindan Nadaradjane (ingénieur)
- Melarkode Akhila (ingénieur)
- Poonam Vishwakarma (ingénieur)



► Peptide cargo adressant un oligonucléotide pour réactiver l'expression de la ferrochelatase

- Madjid Zemmouche (ingénieur)
- Gabriel Falque (ingénieur)

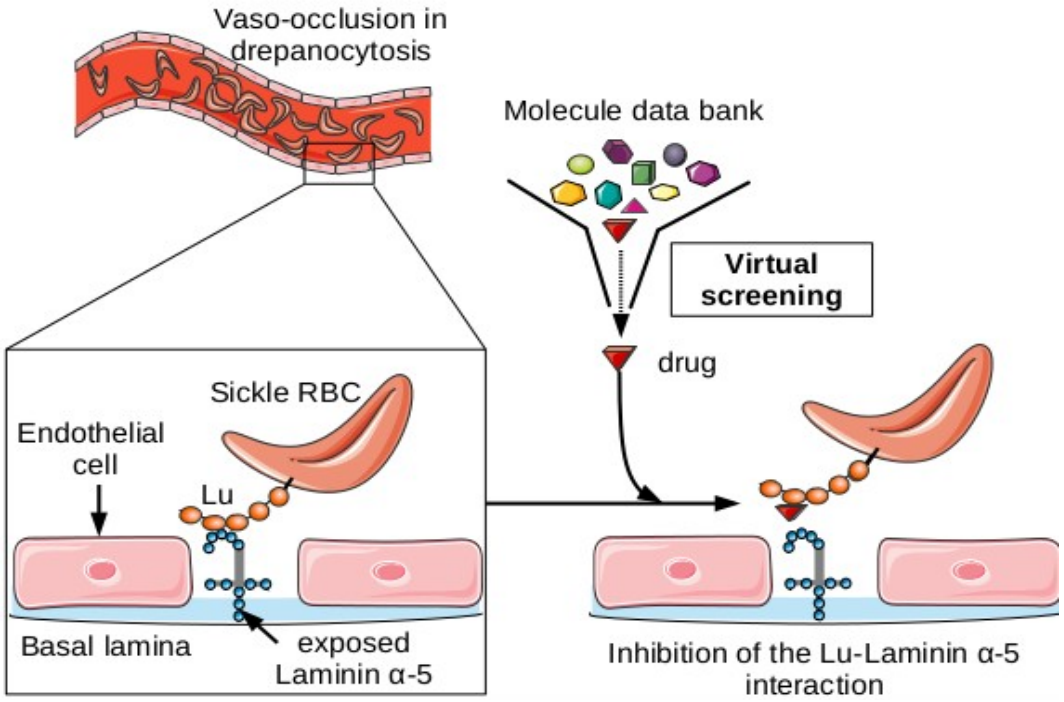
Développer des molécules à visée thérapeutique

Inhibition de l'interaction Lu – Laminine

- Fabrice Gardebien
- Noelly Madeleine (doctorant)
- Guillaume Beck (doctorant)

► Deux brevets (OEB)

► Contrat de Licence d'exploitation avec biotech Hartis-Pharma (collaborations)

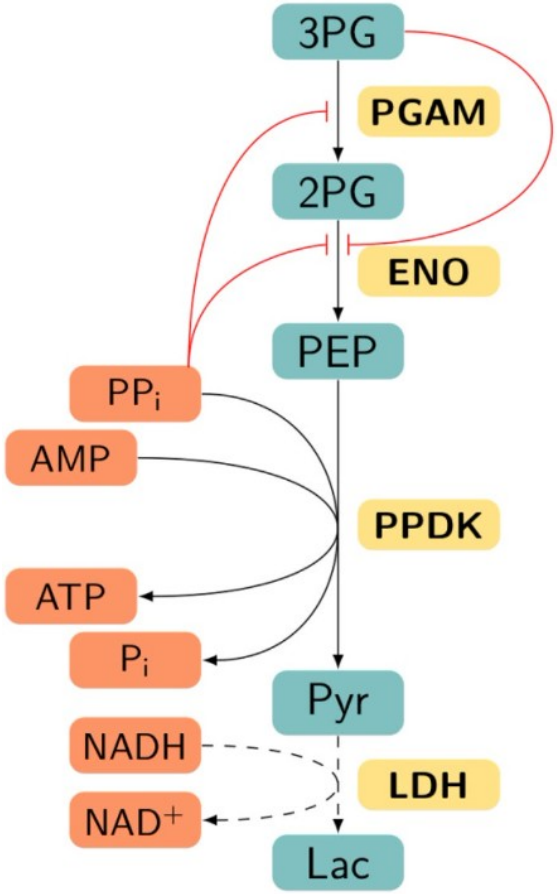


Modéliser des voies métaboliques

Objectif : Comprendre et modéliser les mécanismes de régulation des voies métaboliques.

Méthodes : Approches basées sur les reseaux de neurones et sur les graphes

- Frédéric Cadet,
- Philippe Charton,
- Lo-Thong Ophélie



Apprentissage profond et Approche multimodale

L'apprentissage profond fait référence à des algorithmes de réseaux de neurones artificiels dont le fonctionnement est similaire au réseau de neurones du cerveau humain.
La multimodalité consiste à combiner des données de différente nature (image, son, texte, données « omiques »…) afin d'effectuer une prédiction.
Objectif : Développer et évaluer des architectures des réseaux de neurones pour le traitement de données biologiques.
Exemples d'application : Prédiction des interactions entre molécules (ligands…)
Diagnostic de cancers…

- Frédéric Cadet,
- Philippe Charton,
- Freddy Oulia (doctorant)