MSc in Chemistry and Materials engineering
Master Thesis subjects 2019-2020 proposed by
3BIO-BioInfo
(BioControl, BioInformatics & BioMatter -
Computational Biology and Bioinformatics)

1. Rational design of modified proteins [Marianne Rooman & Fabrizio Pucci]

Proteins carry out a large variety of biological functions in living organisms. Some proteins, for example, act as particularly specific and efficient catalysts. The possibility to exploit the functional properties of proteins in industrial applications (food industry, chemical processes, pharmaceutical developments, etc.) is extremely interesting; however, one of its major limitations is that proteins generally lose their stability and activity under non-physiological conditions. The ability to design modified proteins that remain structured and active at higher (or lower) temperatures is therefore an important objective of both fundamental and industrial research. The project consists in developing efficient and fast computational tools to predict changes in stability, solubility or interactions of proteins upon mutations, which are applicable on a genome-wide scale. This software will be applied to rationally modify proteins of industrial interest and increasing their efficiency within a given application. This theme is part of a spin-off company creation.

2. Prediction of deleterious human genome variants [Marianne Rooman & Fabrizio Pucci]

Next Generation Sequencing produces massive amounts of genome data that are revolutionizing biological and medical research, and paves the way towards personalized medicine. Among the exome variants that lead to amino acid mutations, most are neutral in the sense that they only modify the individual's phenotype, but some are the cause of diseases. The identification of deleterious mutations and their characterization are of prime importance for setting up personalized therapies. The project consists in developing and applying bioinformatics tools to predict disease-causing protein variants and trying to understand why they are so, in terms of protein characteristics such as stability, solubility, flexibility and function. This project will be conducted in the framework of the ULB-VUB (IB)[2] Interuniversity Institute of Bioinformatics in Brussels.

3. Prediction of B-cell epitopes for the rational design of vaccines [Marianne Rooman & Fabrizio Pucci]

Maintaining global health requires the development of generic and versatile technologies that allow fast and effective responses to the large variety of disorders, in particular cancer and emerging infectious diseases. Among these, peptide and protein vaccines play an important role. The *in silico* identification of immunogenic B-cell epitopes on potential antigens, which could be included in vaccines, is thus a challenging goal, and requires the development of reliable B-cell epitope prediction tools. To design such predictors, we will rely on experimentally characterized antibody-antigen complexes, detect informative sequence- and structure-based features, and combine them into a predictor using state-of-the-art machine learning techniques. This project will be realized in collaboration with cancer immunologists.

4. Synthetic gene circuits and noise control [Marianne Rooman & Fabrizio Pucci]

Synthetic biology is a relatively new field whose focus is on improving already existing and engineering new gene circuits. In order to implement a new gene circuit one must understand its behavior in terms of the system parameters. This requires that we understand not only the system's averaged deterministic behavior, but also how random variations, *i.e.* internal and external noise, affect its performance. The project consists in modeling systems of increasing complexity, using stochastic differential equations, and analyzing their noise levels defined as the variance of the number of molecules. We will investigate models of various biological systems, such as prokaryotic and eukaryotic gene regulation and protein oligomerization, and attempt to understand the general relationship between noise, complexity, and some key characteristics of the systems.

5. Study of the dynamics of house dust mite allergens from family 5 [Dimitri Gilis]

House dust mites allergy represents an important public health problem. House dust mite allergens are grouped in several families. Allergens from family 5 are proteins whose biological function is still unknown, as well as how they provoke allergy. They show a three-helix bundle, and some of them are monomers, whereas others are dimers. In the dimers, one of the helices is kinked, and a hydrophobic cavity that could accommodate a ligand is observed. The relationships between these structural features and the allergenic properties of these allergens are also unknown.

We propose to study by molecular dynamics methods the influence of mutations and of solvent conditions on the dynamics of these allergens.

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