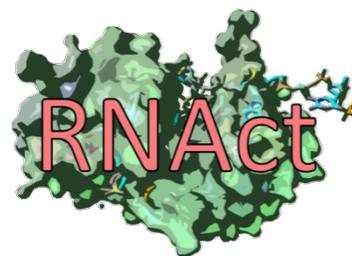# Predicting biophysical characteristics of proteins from their amino acid sequence.

Domain: Structural bioinformatics; computational biology; methods development; machine learning

**Keywords**: protein sequence-based prediction; protein design; protein biophysics

Promotor: Wim Vranken (http://we.vub.ac.be/nl/wim-vranken; http://bio2byte.be/people/2)

Starting date: 1st of September 2019, for a period of 3 + 1 years

Location: Bio2Byte group (http://bio2byte.be/); (IB)² (http://ibsquare.be/); VUB, Brussels, Belgium.

Funding: H2020-MSC-ITN project RNAct (http://rnact.eu/)

In this Ph.D. project, you will further develop protein sequence-based prediction approaches from estimations of dynamics and conformation directly from experimental NMR data on proteins, similar to DynaMine (http://dynamine.ibsquare.be). These estimations can encompass the whole range of protein behaviour, from intrinsically disordered via molten globule to fully folded, and reflect the actual behaviour of the protein solution. We have evidence that such predictions capture the 'emergent properties' of proteins, and add a biophysical dimension to the protein sequence.
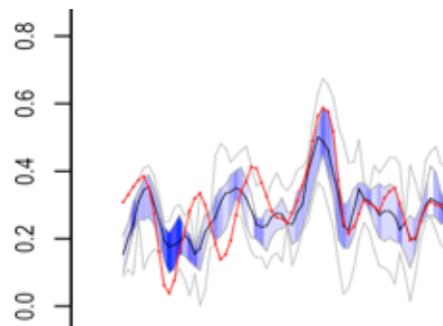
We intend to incorporate these predictions of emergent protein properties in computational pipelines for protein design, more specifically the design of RNA recognition motif (RRM) proteins. These RRMs are very flexible, and it is essential to include their dynamics in any design approach.

Besides the work in Brussels, you will spend a 3 month secondment at the CSIC (Valencia, Spain) to learn about incorporating molecular information in pathway modelling for synthetic biology.

The project is part of a computational/experimental EU MSCA-ITN project with a total of 10 Ph.D. students, and is highly interdisciplinary. Good programming skills (preferentially Python and/or C++) are essential, with knowledge of machine learning/artificial intelligence very desirable, and skills in discrete mathematics and statistics much appreciated. A background knowledge of (structural) biology is a bonus. Candidates must be motivated to learn about all disciplines relevant to the project.

Candidates must be fluent in English.

Further information: http://rnact.eu

Contact and information: e-mail to info@rnact.eu

Applications must be submitted online at https://tinyurl.com/rnact-eu, select ESR1.

Eligibility conditions apply, check the application website.

Deadline for applications: 15/03/2019.