Project proposal

Project title	Prediction of homodimer interaction sites and evaluation of their dissociation potential
First Supervisor	Dr — Jean-Christophe Nebel
Second Supervisor	Prof Declan Naughton
School	Computing and Information Systems
Other member of supervisory team (no more than three KU supervisors in total)	
Specific requirements beyond 2:1 degree	

Project summary

(max 4,000 characters)

MSc by Research

Interactions between proteins are important for many biological functions and play a fundamental role in the immune system. Unfortunately, most protein-protein interactions are largely unknown.
Most known interactions happen between pairs of identical proteins, called homodimers. Although their mode of interaction varies, preliminary analysis of protein 3D structure suggests the symmetrical, or head-to-tail, configuration is particularly frequent. Therefore, recognition of patterns predicting head-to-tail configurations could lead to the automatic prediction of homodimers. Moreover, quantification of the stability of this particular binding mode would inform regarding its ability to allow dimer dissociation which is required by many signalling pathways.
The aim of this project is, first, to apply machine learning techniques to analyse known protein interactions in a head-to-tail configuration in order to discover specific patterns. Second, binding descriptors will be designed to allow automatic detection of potential homodimer interaction sites.

Finally, the strength of those sites will be quantified to assess their stability. This work will be applied to human defensins whose internalisation is expected to require dissociation of their dimer form.