Title: Improving fragment assembly protein structure prediction

Abstract: Protein structures can elucidate functional understanding, explain disease mechanisms and inform drug design. However, experimental structure determination is costly, and technically difficult and while the three-dimensional structure of proteins is difficult to obtain amino acid sequences are easily available and far outnumber solved structures. However, current de novo protein structure prediction methods are heuristics limited by the enormous search space, with successful prediction largely restricted to small, single domain proteins.

The three key components of de novo fragment-assembly methods for protein structure prediction are the fragment library, the "energy" function and the search method. In this talk I will give an overview of my groups work on improving each of these stages. Firstly, describing the development of a novel fragment library Flib that uses predicted secondary structure to determine library generation strategy [1]. Secondly, giving a comparison of the different co-evolution contact predictors in terms of their ability to improve protein structure prediction [2]. Finally demonstrating how sequential prediction approaches using SAINT2 can improve both search heuristics and final model quality.

[1] Saulo Henrique Pires de Oliveira, Jiye Shi, Charlotte M Deane, Building a better fragment library for de novo protein structure prediction, Plos One, 2015, 10(4), e0123998

[2] Saulo Henrique Pires de Oliveira, Jiye Shi, Charlotte M Deane, Comparing co-evolution methods and their application to template-free protein structure prediction, Bioinformatics, 2017; 33 (3): 373-381. doi: 10.1093/bioinformatics/btw618