Protein structures are valuable tools for understanding protein function. However, protein structures are often considered as rigid bodies while protein dynamics is a key element in protein function. Full understanding of protein function at the molecular level requires accounting for protein flexibility.

Protein structure can be described by a limited set of recurring local structures. We established a library composed of 120 overlapping long structural prototypes (LSPs) representing fragments of 11 residues in length and covering all known local protein structures. We developed a prediction method that proposes structural candidates in terms of LSPs along a given sequence (Bornot et al., Proteins, 2009). We utilized this methodology to predict protein flexibility.

X-ray structure coordinates do not necessarily reflect all the diversity of conformations adopted by proteins in cells. On the other hand, X-ray B-factors are considered as good indicators of flexibility. Alternatively, molecular dynamics simulations (MD) are used in routine to account for dynamics. So we performed MD on a set of proteins.

We examine flexibility according two different descriptors, root mean square fluctuations and B-factors. We define three flexibility classes and propose a method based on the LSP prediction method for predicting flexibility along the sequence. This method competes rather efficiently with the most recent, cutting-edge methods based on true flexibility data learning with sophisticated algorithms (Bornot et al., Proteins, 2011). Flexibility prediction correlates well with disorder prediction.