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Abstract

Investigating the Structure-Dynamics-Function Relationship in Antibodies †

Marta Rigoli

Physics Department, University of Trento, Trento, Italy

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The paradigm that connects sequence, structure and function in proteins has been revisited in recent years, opening new perspectives on the importance of dynamics [1]. In this work we tackle this issue through the analysis of all-atom molecular dynamics (MD) simulations, with the final objective of correlating motions and structural features. We first characterize the dynamics of an antibody, through 2 μs of all-atom molecular dynamics simulations, to investigate the correlation between structural features and the flexibility of the molecule. Subsequently we perform 2 μs of all-atom MD simulations of the same antibody bound to its antigen, to investigate the changes in dynamics [2].

We analyzed the simulations through various different techniques among which we highlight the power of those based on the calculation of the information transfer between different amino acids [3]. These types of measurements allow us to identify significant correlations among protein regions, providing clues on the mechanism of protein function. The investigations carried out in this work also serve as a guide in the identification of those structural patterns whose preservation is necessary in the construction of coarse-grained models. Overall this study is meant as a starting point for the application of a multi-scale method to biologically relevant macromolecules.

References

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