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Abstract

Modelling of Protein–Polyphenol Interactions †

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Abstract: The interaction between proteins and polyphenols is known to modify both the bioavailability and bioactivity of dietary polyphenols. Understanding these interactions can facilitate the design of delivery systems for polyphenols in the digestive tract. Molecular modelling of protein–polyphenol and protein–ligand interactions in general has long been used as a way to identify small molecule binding sites on proteins. However, these are often used without a careful consideration of the assumptions used and limitations of these methods, and how this affects the accuracy of the predictions. In this paper, two common methods for predicting binding site location and binding energy, molecular dynamics simulation and molecular docking, will be discussed. The simplifications and assumptions implicit in these approaches, as well as ways to improve their predictions will be covered.

Keywords: molecular modelling; molecular dynamics simulation; molecular docking

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