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Molecular simulations for investigating the role of food polyphenols

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Food components are object of many studies aimed to identify compounds responsible of positive effects in nutrition and food science. Compound categories include antioxidants, whose positive activity is commonly related to their activity in deactivating free radicals. Polyphenols are of particular interest, and studies demonstrate many positive effects [1]. We have recently investigated the role of apple polyphenols [2], in particular for the effects reported in literature in the past years [3-4], and we evidenced possible protein targets for polyphenols found in apple but present also in other fruits and vegetables. Our results open the perspective of identifying metabolic pathways affected by polyphenols. To this aim, we are investigating in more detail the potential protein targets already identified in our study, and defining the possible role of each compound investigated in the modulation of the related target activity. This ongoing study is based on the integration of techniques and resources previously used in our studies [2, 5-7], as molecular simulations of protein-ligand docking, mutation effects, pathways analysis, and online bioinformatics resources for collecting information about proteins and their structural and functional properties.

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