Computational investigation on the carbohydrate binding site of Frutalin

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Frutalin is a tetrameric carbohydrate-binding protein obtained from breadfruit seeds [1]. Biomedical interest on frutalin comes from the high affinity exhibited by these molecules toward carbohydrates expressed by specific tumor cells[2]. So far, no theoretical computational studies have been carried out to investigate the binding characteristics of frutalin, which is probably due to the large number of atoms that should to be considered for *in silico* calculations. We investigate the binding of frutalin [1] with specific carbohydrate molecules [3] using a theoretical "cut-model", considering only the carbohydrate binding site[4]. The spatial cuttings are performed with radius 4, 5 and 6 Å around the center of the carbohydrate ligand, including the aminoacids present in this region. We use the Carr-Parrinelo Augmented Plane Wave (CP-PAW) method[5,6], which is an ab-initio all-electron reciprocal space method based on Kohn-Sham scheme of the density functional theory (DFT)[7]. The investigation of this very complex problem, can be divided into 3 main steps. In the first step, we study the electronic structure and structural properties of four isolated carbohydrates: A-D-Galactose, A-D-Mannose, A-D-Glucose and Lactose. In the second step, we study the isolated binding site of the protein and in a third step we investigate the interaction of the protein with each carbohydrate. Our theoretical results are compared with available measurements in each step. The study of the isolated carbohydrates allows us to demonstrate that our methodology is well suited to predict the electronic properties for carbohydrates since we found a very good agreement with experimental results[3]. Also our model for the protein is validated through comparison with UV spectroscopy and for this a semi-empirical theoretical calculation is done. The investigation of the third step is now in progress.

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