Computational Biology and Gastronomy research in the Food and Nutrition Torribera Campus.

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Computational biology: The family of concentrative Na^+/nucleoside cotransporters in humans is constituted by three subtypes, namely, hCNT1, hCNT2, and hCNT3. Besides their different nucleoside selectivity, hCNT1 and hCNT2 have a Na^+/nucleoside stoichiometry of 1:1, while for hCNT3 it is 2:1. To date, their three-dimensional structures remain unknown and the residues implicated in Na^+ binding are unclear. We have identified and characterized the Na^+ binding sites of hCNT3 by combining molecular modelling and mutagenesis studies. A model of the transporter was obtained by homology modelling, and key residues of two sodium-binding sites were identified and verified with a mutagenesis strategy. Furthermore, the structural model explains the altered sodium-binding properties of the hCNT3C602R polymorphic variant and supports previously generated data identifying the determinant residues of nucleoside selectivity.

Computational Gastronomy: The increasing accumulated data in different disciplines has led to the emergence of *Big Data analysis* tools and applications focused to extract valuable information from the huge amount of data available. One of the new fields that might benefit from this in a health-oriented perspective is gastronomy, as the amount of available data in the field is rapidly increasing. Computational gastronomy is emerging as a new discipline focused on the study of gastronomic data with computational tools that has already been used to test hypothesis or make new predictions. We have started projects based on this emerging discipline and oriented to compare corpus of recipes. Our goal is to be able to use gastronomic data to work in food-drug interaction projects and other health related projects.

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