Title: **Computational analysis of the active center of carbohydrate-degrading enzymes: retaining glucosidases**

Student: Marc Muñoz Ferras

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Supervisor/s: Dra. Carme Rovira Virgili
Departament of Organic Chemistry

Glycoside hydrolases (GH) are highly specific enzymes that catalyze the hydrolysis and formation of the glycosidic bonds in polysaccharides, respectively. They can be found in all domains of life from bacteria to a multicellular organism like humans. The study of their structure and behavior is very important since a non-activity of GH enzyme can lead to very common diseases such as lactose intolerance, diabetes, or neurological disorders.

The enzyme studied in this project is a GH 79-β-glucosidase from *Acidobacterium capsulatum*. β- Glucuronidase is a family of enzymes that hydrolysis β-D-Glucuronic acid residues Glucuronic acid which is a component of proteoglycans and are responsible of genetic disorders related to cancer.

This study will be performed in computational analysis by combining classic and density-functional theory (DFT) methods.

Computational studies allow research groups to study molecules properties while saving an important amount of time and resources. In a GH catalysis mechanism acid/base and nucleophile residues are required, so by studying the protonation state of the residues involved in the catalysis and their interaction with the disaccharide, it is possible to understand the impact of the pH value in the reaction.

Keywords: glycoside hydrolase, GH79 β-glucosidase, Molecular dynamics simulation, retaining mechanism