Séminaire de Chimie Théorique

Salle de conférences, 3ème Est, Bat. A12
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Understanding physico-chemical, biological and optical properties of natural compounds at the molecular scale

Quantum calculations (mainly DFT) and molecular dynamics are very powerful tools to evaluate the physico-chemical properties of natural compounds in order to rationalize their biological/optical properties and to predict their pharmaceutical properties. Here we summarize the different topics that have been studied over the past decade in our group and in collaboration with both experimentalists and theoreticians.

Antioxidant Activities.[1-9] Thermodynamic parameters (mainly bond dissociation enthalpies (BDE) of the O-H phenolic bond) allow us to accurately predict the antioxidant capacities of natural and hemi-synthetic compounds. Based on the Transition State and the Marcus Theories, kinetics is also evaluated providing a better prediction of the antioxidant behaviour in solution or in the organism.

Chemistry and synthesis.[10-12] Quantum chemistry is also powerful to better understand bio-inspired chemical synthesis. The calculations performed in our group support experimental data (e.g., dimerisation, conjugation). Thermodynamic and kinetic calculations fully explain regio- and stereo-selectivity, showing in many cases importance of H-bond and p-stacking.

Interaction with Lipid Bilayer Membranes.[13-14] Numerous projects are developed to provide an accurate picture of the interaction between natural compounds with membranes (polyphenols and other p-conjugated derivatives of pharmaceutical interest). Molecular dynamics allows evaluation of the ability of these molecules to approach the membrane and to predict their "exact" location and orientation.

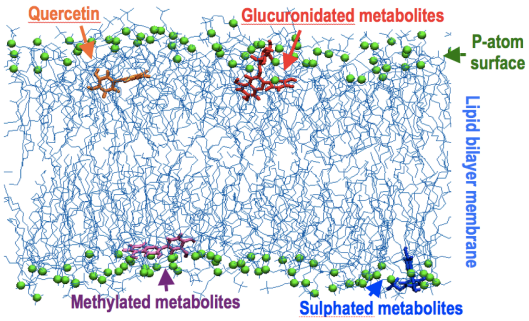

Fig. 1: Insertion of polyphenols in lipid-bilayer membranes

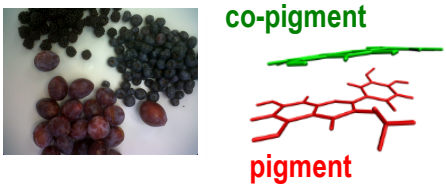

Fig. 2: Copigmentation complexes

Pigmentation and optical properties.[15-18] TD-DFT is a very effective tool to reproduce the capacity of natural polyphenols to absorb UV/Vis. light. The accurate prediction of spectroscopic shifts and modulation of oscillator strength helps understanding of pigmentation and co-pigmentation (mainly driven by p-stacking interaction).

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