Theoretical Exploration of the Photosensitization Properties in Porphyrin-Cellulose based Materials with Antibacterial Applications

Gloria Cárdenas-Jirón[1], Cristhy Gonzalez[1]

[1]*Laboratorio de Química Teórica, Facultad de Química y Biología, Universidad de Santiago de Chile (USACH), Casilla 40, Correo 33, Santiago, CHILE*
E-mail: gloria.cardenas@usach.cl

Materials with antibacterial properties are of interest in a wide range of fields such as food packing and handling of medical items, between others, and several experimental studies are being focused on antibacterial surfaces. Porphyrins are macrocycles with excellent photosensitization properties because they absorb light at visible wavelength producing a singlet excited state that decays to the first triplet excited state. The phototoxic effects of porphyrins depend on the formation of singlet oxygen, yielded after the decay of the first triplet excited state to the ground state, that leads to cell death. At the experimental level, much work has been performed to look for the best photosensitizers. Porphyrins covalently linked to cellulose via a triazine derivative have recently been synthesized and proposed as polymer material for antimicrobial applications. However, it is still not clear how is the molecular binding between these species.

The aim of this work is to explore the binding porphyrin-cellulose and determine how this affects the photosensitization properties of porphyrin. In that way, we studied at the density functional level of theory a set of conformations where porphyrin is bounded by a triazine ring to a tetramer of cellobiose in a *top*, *inner* and *outer* side. For each conformation, we studied the electronic excited states and characterize the porphyrin bands such as Soret and Q bands in terms of the molecular orbitals. The more relevant result obtained is that the porphyrin does not lose the photosensitization properties but the position of the binding denotes changes in the absorption bands. The study shows that is possible to design an antibacterial material based in cellulose where the photosensitization properties can be tunable.

Acknowledgements. Financial support of project FONDECYT/CHILE N°1131002 is greatly appreciated.